

CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 19 SEPTEMBER 2007.

NEWS HOURS      STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN      Welcome Banner and News Items  
NEWS IPC8      For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

FILE 'HOME' ENTERED AT 17:25:32 ON 28 JAN 2008

FILE 'REGISTRY' ENTERED AT 17:25:47 ON 28 JAN 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 27 JAN 2008 HIGHEST RN 1000849-38-6  
DICTIONARY FILE UPDATES: 27 JAN 2008 HIGHEST RN 1000849-38-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

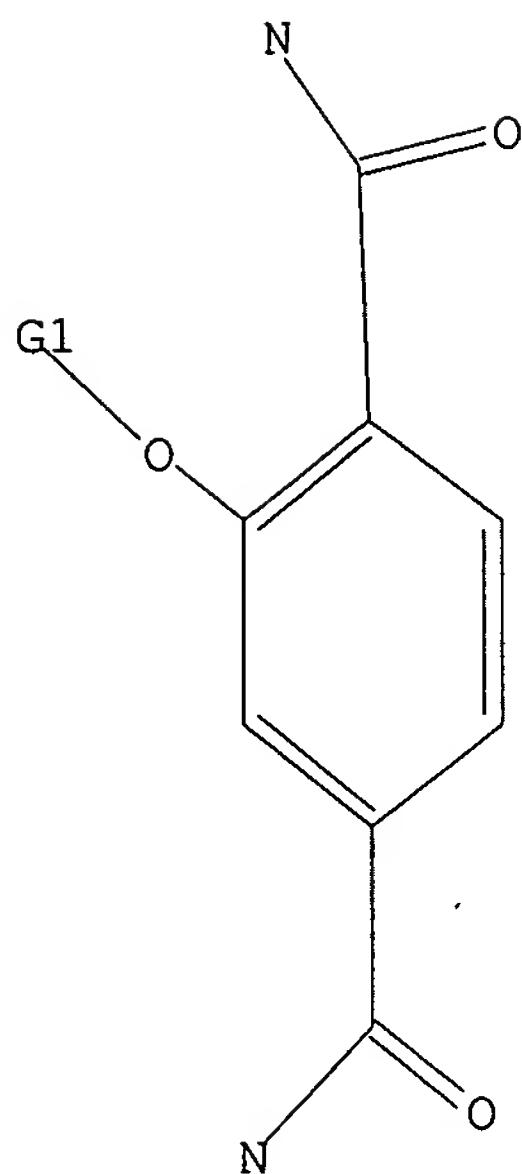
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=> Uploading C:\Documents and Settings\jcho2\My Documents\10588478-a.str

L1 STRUCTURE UPLOADED

=> d 11  
L1 HAS NO ANSWERS  
L1 STR



G1 Ak,Cy

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss sam
SAMPLE SEARCH INITIATED 17:26:07 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 173 TO ITERATE

100.0% PROCESSED 173 ITERATIONS 22 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 2671 TO 4249
PROJECTED ANSWERS: 159 TO 721

L2 22 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 17:26:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 3389 TO ITERATE

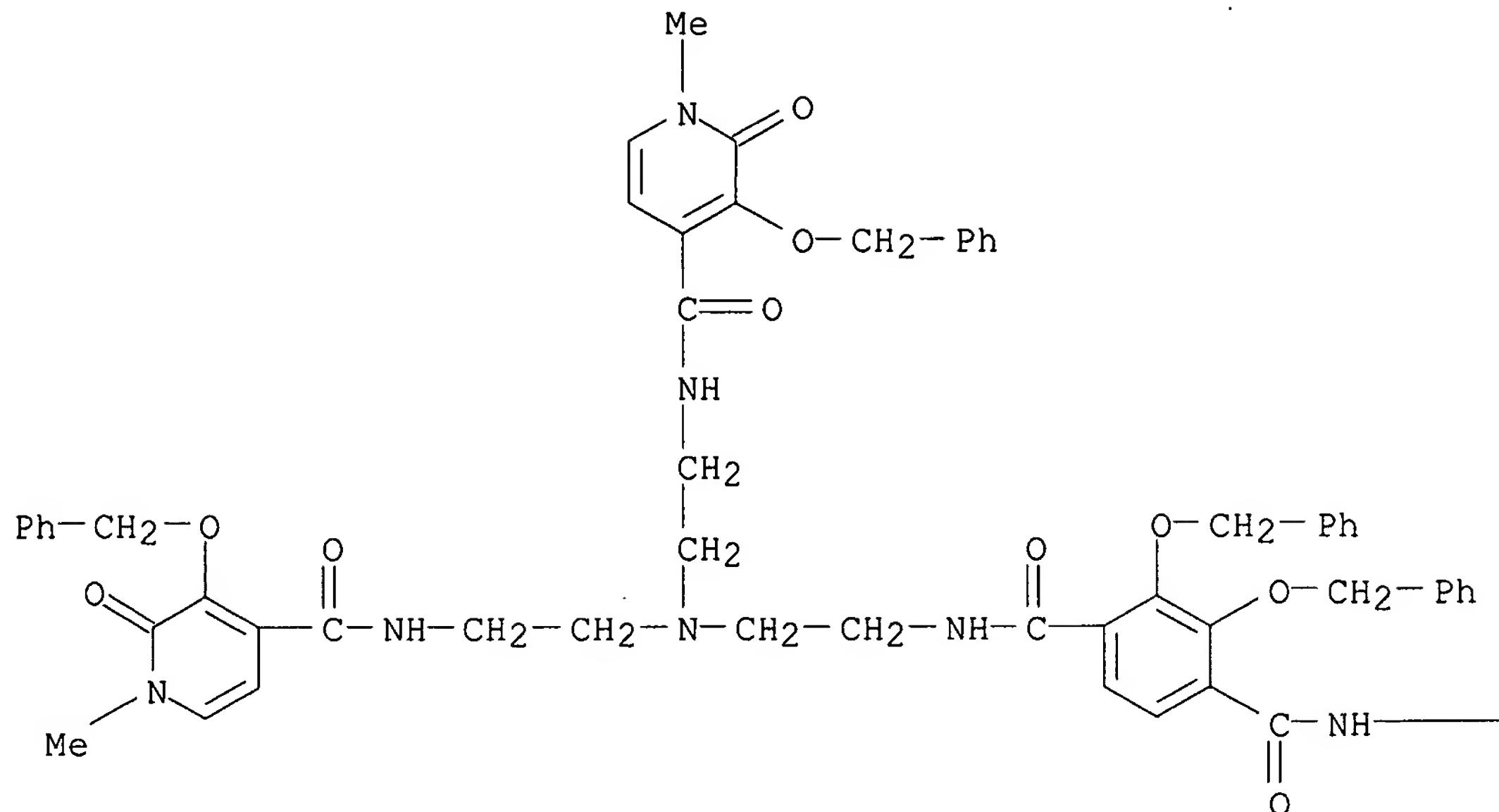
100.0% PROCESSED 3389 ITERATIONS 564 ANSWERS
SEARCH TIME: 00.00.01

L3 564 SEA SSS FUL L1

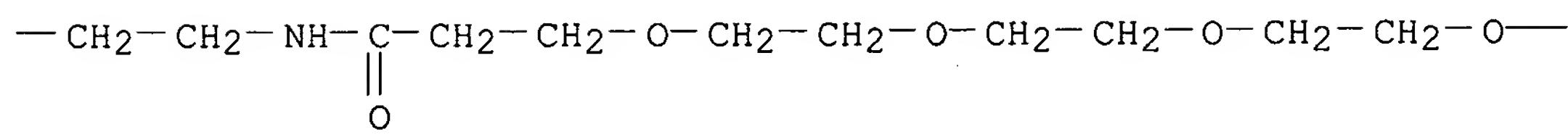
=> d scan

L3 564 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN
IN 1,4-Benzenedicarboxamide, N-[2-[bis[2-[[1,2-dihydro-1-methyl-2-oxo-3-
(phenylmethoxy)-4-pyridinyl]carbonyl]amino]ethyl]amino]ethyl]-N'-(4-oxo-
7,10,13,16,19,22,25,28,31,34,37,40-dodecaoxa-3-azahentetracont-1-y1)-2,3-
bis(phenylmethoxy)- (9CI)
MF C84 H112 N8 O23
```

PAGE 1-A



PAGE 1-B



PAGE 1-C

— CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—————

PAGE 1-D

— CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—O—CH<sub>2</sub>—CH<sub>2</sub>—OMe

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=>  
Uploading C:\Documents and Settings\jcho2\My Documents\10588478-b.str

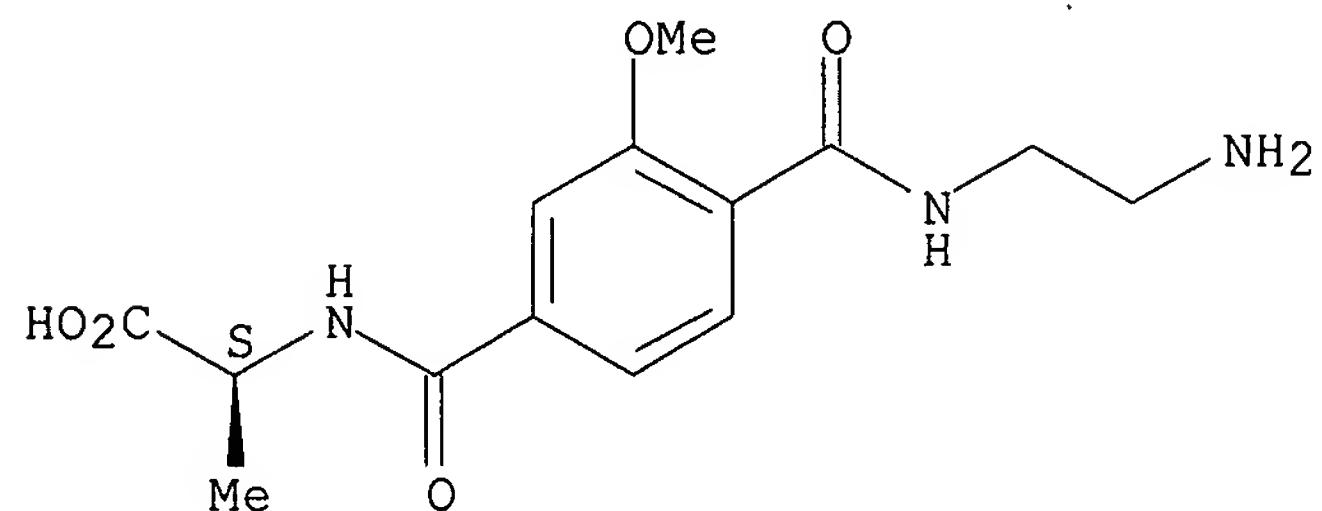
L4       STRUCTURE UPLOADED

=> d 12

L2   ANSWER 1 OF 22   REGISTRY   COPYRIGHT 2008 ACS on STN  
RN   919772-33-1   REGISTRY  
ED   Entered STN:  07 Feb 2007  
CN   L-Alanine, N-[4-[(2-aminoethyl)amino]carbonyl]-3-methoxybenzoyl]- (CA

INDEX NAME)  
FS STEREOSEARCH  
MF C14 H19 N3 O5  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL

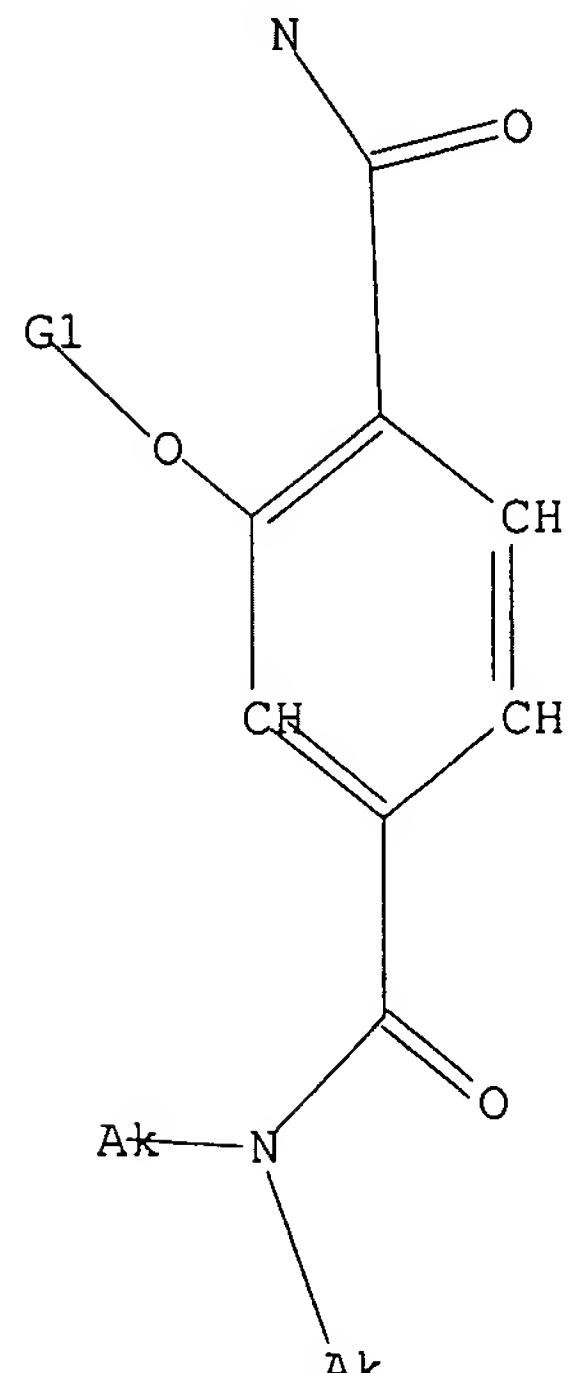
Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> d 14  
L4 HAS NO ANSWERS  
L4 STR



G1 Ak,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s 14 sss sam  
SAMPLE SEARCH INITIATED 17:31:42 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED -

173 TO ITERATE

100.0% PROCESSED 173 ITERATIONS  
SEARCH TIME: 00.00.01

0 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 2671 TO 4249  
PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s 14 sss full  
FULL SEARCH INITIATED 17:31:48 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 3389 TO ITERATE

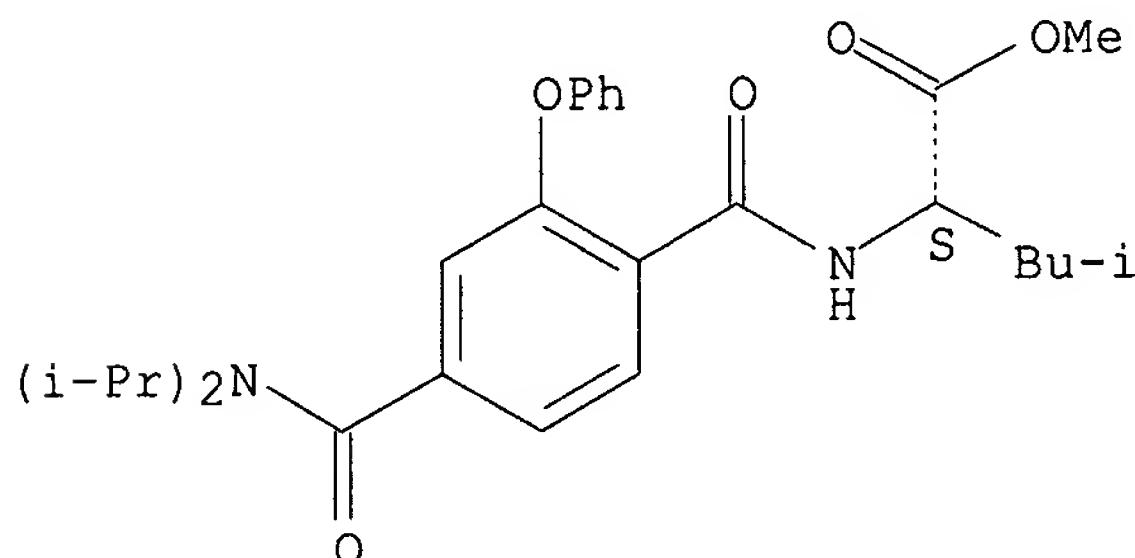
100.0% PROCESSED 3389 ITERATIONS 27 ANSWERS  
SEARCH TIME: 00.00.01

L6 27 SEA SSS FUL L4

=> d scan

L6 27 ANSWERS REGISTRY COPYRIGHT 2008 ACS on STN  
IN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-,  
methyl ester  
MF C27 H36 N2 O5

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):end

=> file caplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 362.86 363.07

FILE 'CAPLUS' ENTERED AT 17:32:05 ON 28 JAN 2008  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the

American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 28 Jan 2008 VOL 148 ISS 5  
FILE LAST UPDATED: 27 Jan 2008 (20080127/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.  
They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 16  
L7 4 L6

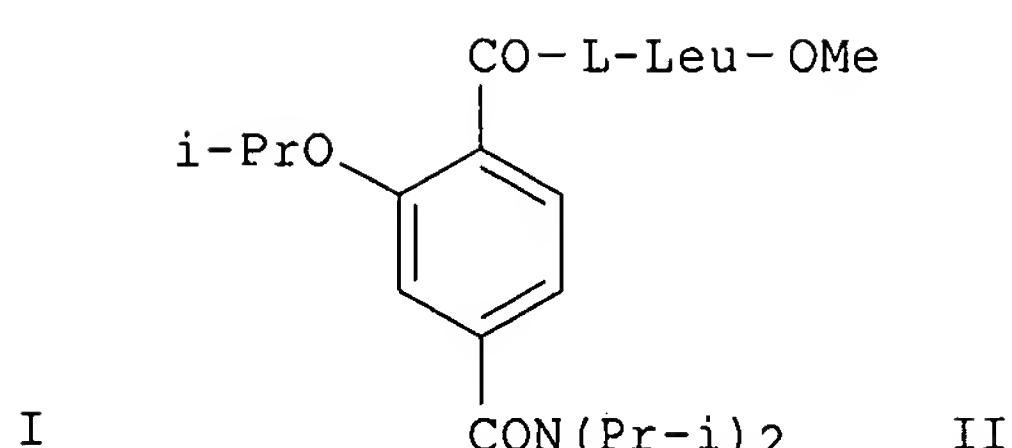
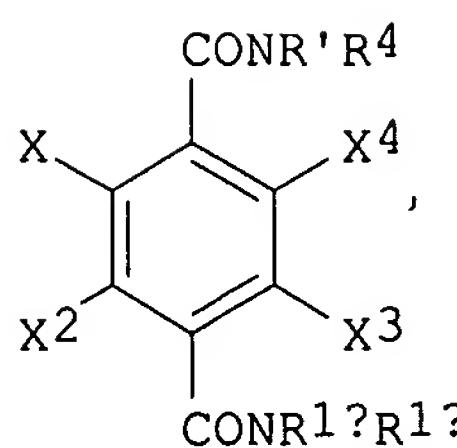
=> d 17 1-4 bib abs hitstr

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 2005:961964 CAPLUS  
DN 143:248664  
TI Preparation of terephthalamide peptidomimetic compounds for therapeutic use  
IN Hamilton, Andrew D.; Yin, Hang  
PA Yale University, USA  
SO PCT Int. Appl., 48 pp.  
CODEN: PIXXD2

DT Patent  
LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005079541	A2	20050901	WO 2005-US5557	20050222
	WO 2005079541	A3	20051103		
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	AU 2005215051	A1	20050901	AU 2005-215051	20050222
	CA 2556447	A1	20050901	CA 2005-2556447	20050222
	EP 1723100	A2	20061122	EP 2005-713917	20050222
	R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU				
	US 2007123592	A1	20070531	US 2006-588478	20061002
PRAI	US 2004-546111P	P	20040219		
	WO 2005-US5557	W	20050222		
OS	CASREACT 143:248664; MARPAT 143:248664				
GI					



**AB** The invention relates to compds. and pharmaceutical compns. based on terephthalamide which are proteomimetic and methods for inhibiting the interaction of an  $\alpha$ -helical protein with another protein or binding site and for treating diseases or conditions which are modulated through these interactions. Compds. I [X is H, halo, R, OR, SR or an amino group, where R is H, (un)substituted alkyl, acyl, aryl, heteroaryl, alkylenearyl or alkyleneheteroaryl; X<sub>2</sub>, X<sub>3</sub>, X<sub>4</sub> are independently H, halo, OH, R<sub>c</sub>, OR<sub>c</sub>, where R<sub>c</sub> is (un)substituted alkyl, acyl, aryl or alkylenearyl; R<sub>4</sub> is H, (un)substituted alkyl, alkenyl or alkylene amine; R', R<sub>1a</sub>, R<sub>1b</sub> are any group given for R<sub>4</sub> or (CH<sub>2</sub>)<sub>0-2</sub>CHR<sub>2</sub>CO<sub>2</sub>H or an alkyl ester, where R<sub>2</sub> is independently H or (un)substituted hydrocarbon, alkoxy, ester, alkanol, alkanoic acid, amine, etc.; or N-R' or NR<sub>1a</sub>R<sub>1b</sub> form an amino acid residue] are claimed. Thus, peptidomimetic compound II, prepared via coupling reaction of L-leucine Me ester hydrochloride, showed inhibitory constant K<sub>i</sub> = 0.781  $\pm$  0.070  $\mu$ M in a fluorescence polarization assay (binding affinity for Bcl-XL).

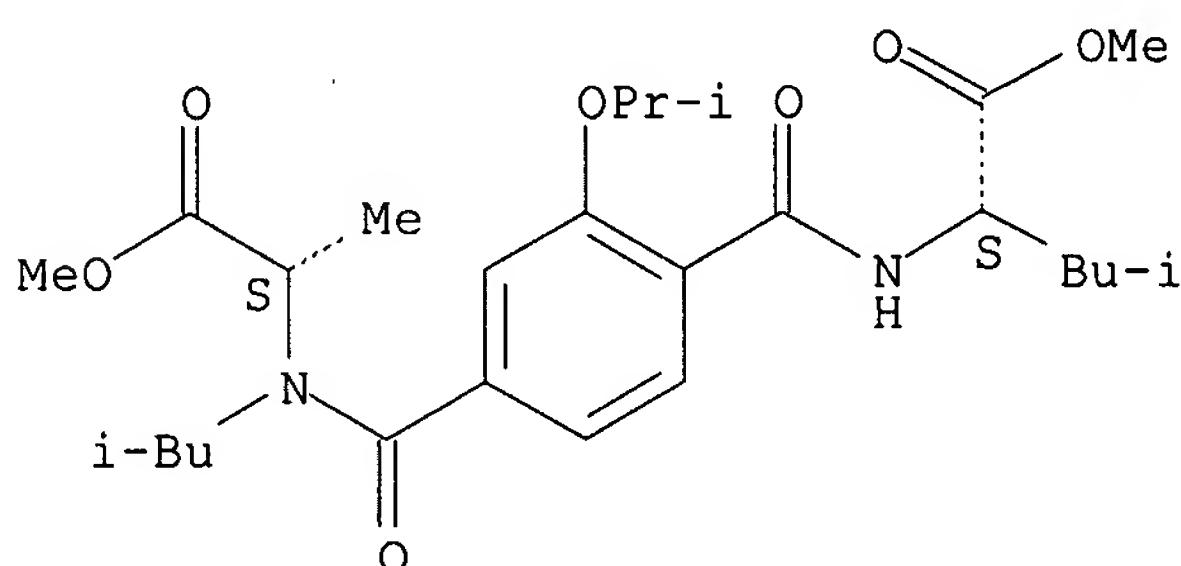
**IT** 681466-00-2P

RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(conformation; preparation of terephthalamide peptidomimetic compds. for therapeutic use)

**RN** 681466-00-2 CAPLUS

**CN** L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



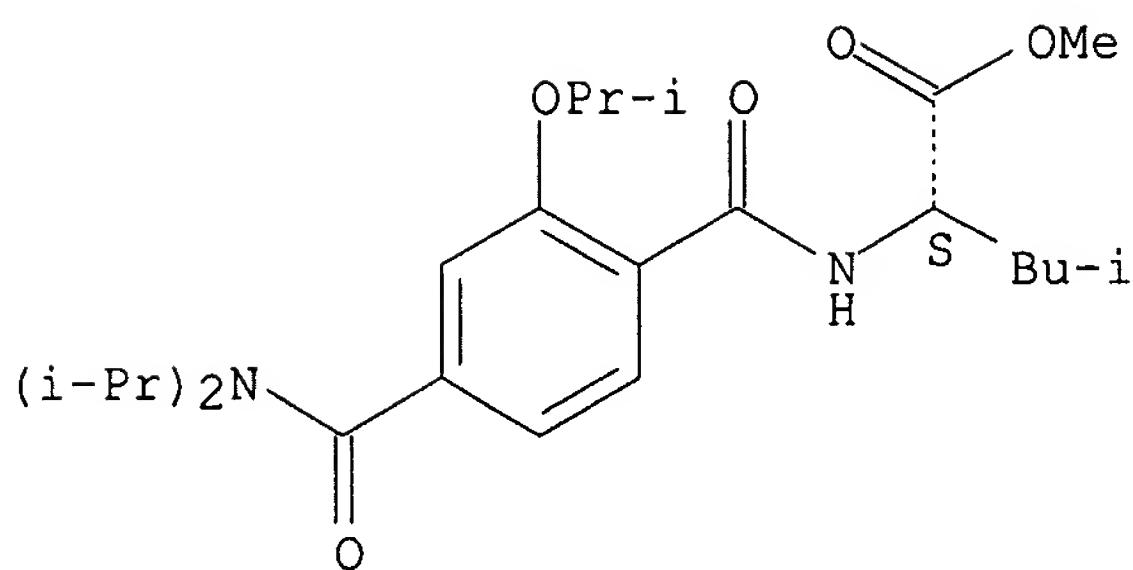
**IT** 681465-54-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of terephthalamide peptidomimetic compds. for therapeutic use)

**RN** 681465-54-3 CAPLUS

**CN** L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-60-1P 681465-62-3P  
 681465-64-5P 681465-66-7P 681465-68-9P  
 681465-70-3P 681465-74-7P 852065-21-5P  
 852065-22-6P 852065-23-7P 852065-25-9P  
 852065-26-0P 852065-27-1P 852065-28-2P  
 852065-29-3P 852065-30-6P 852065-31-7P  
 852065-32-8P 852065-33-9P

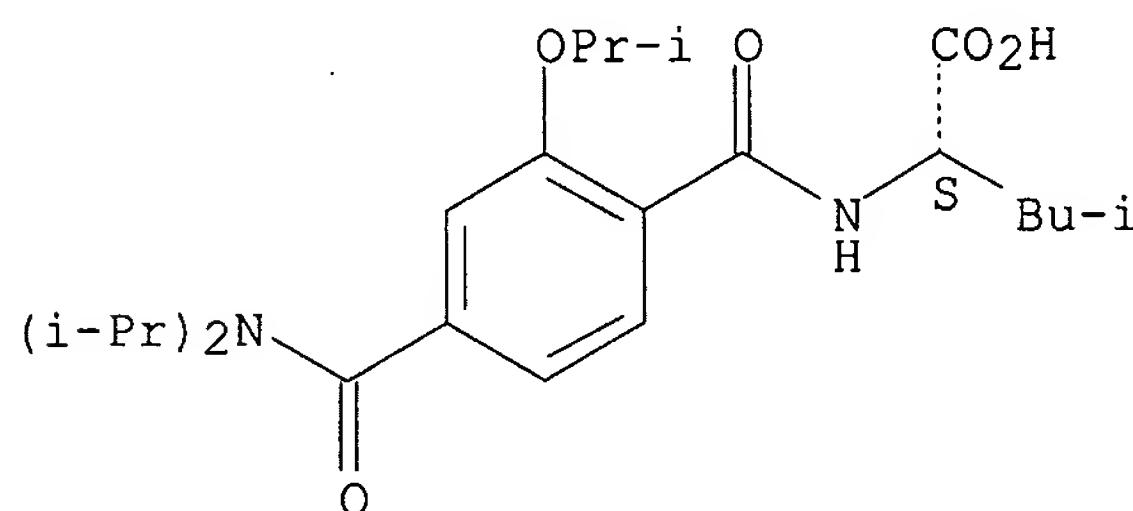
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of terephthalamide peptidomimetic compds. for therapeutic use)

RN 681465-56-5 CAPLUS

CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

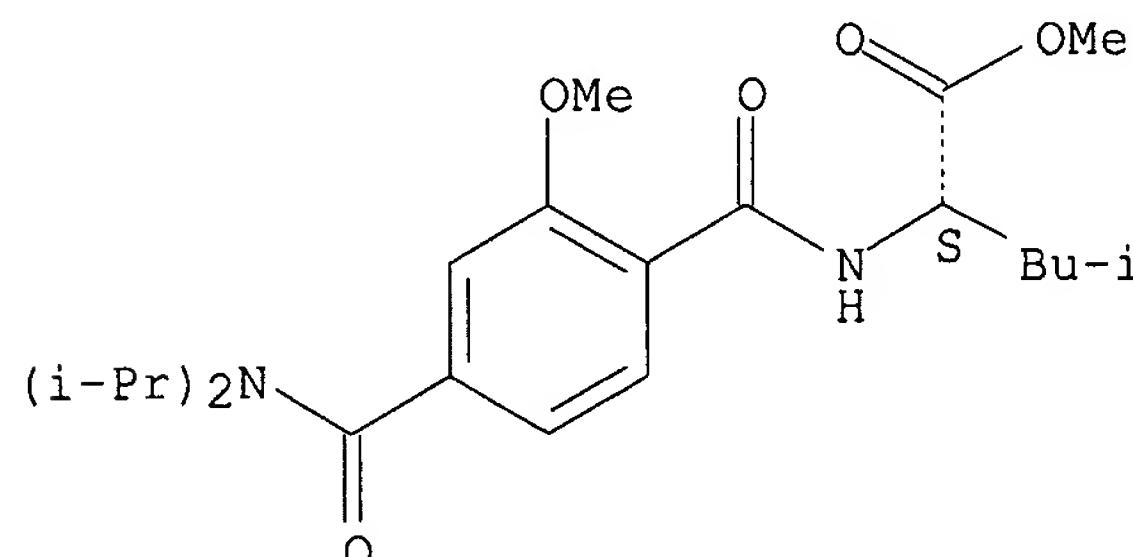
Absolute stereochemistry.



RN 681465-60-1 CAPLUS

CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

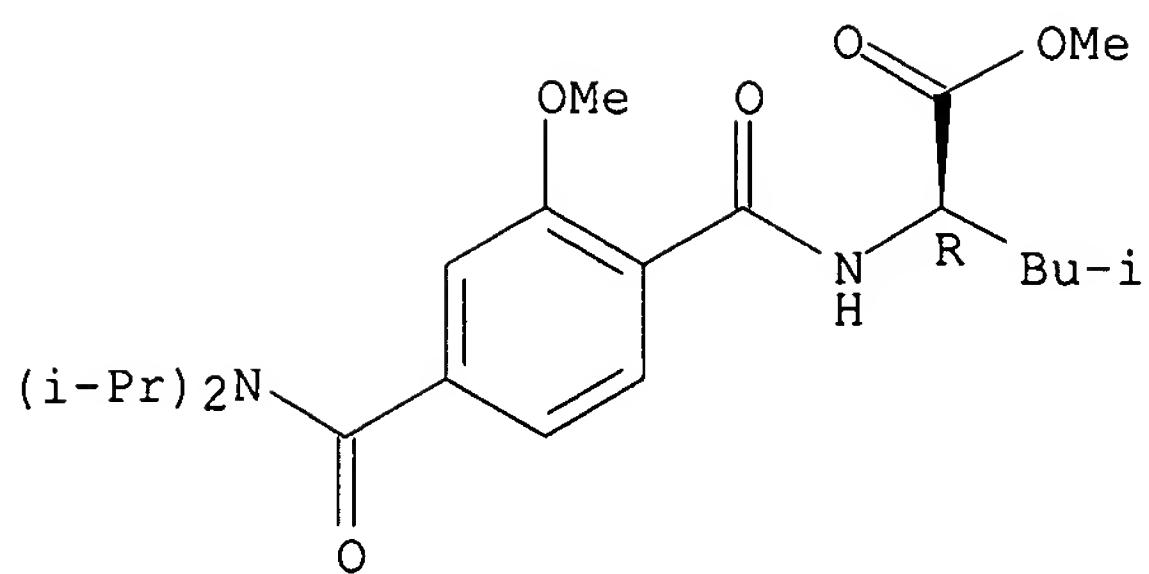
Absolute stereochemistry. Rotation (-).



RN 681465-62-3 CAPLUS

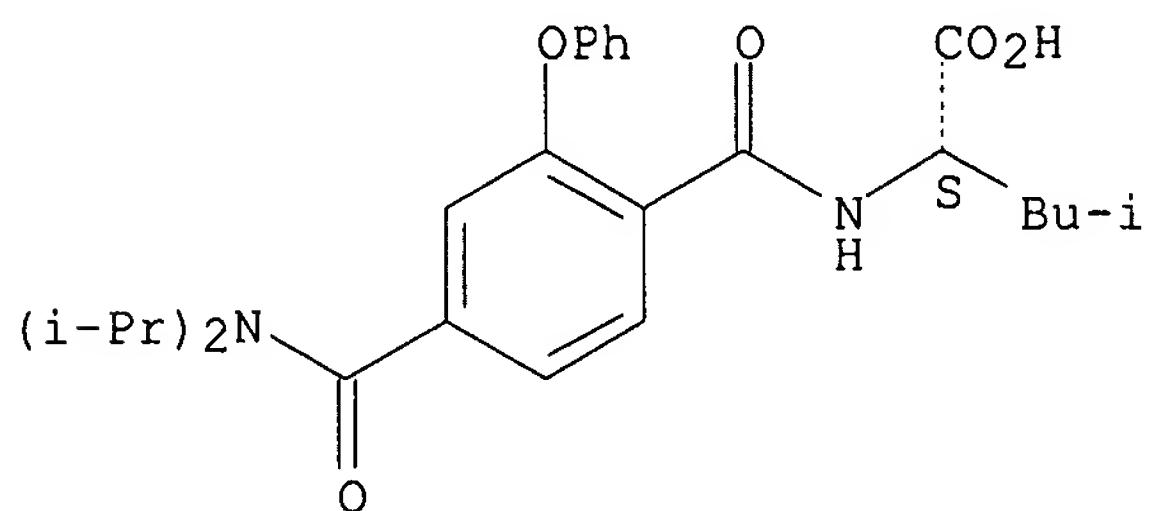
CN D-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



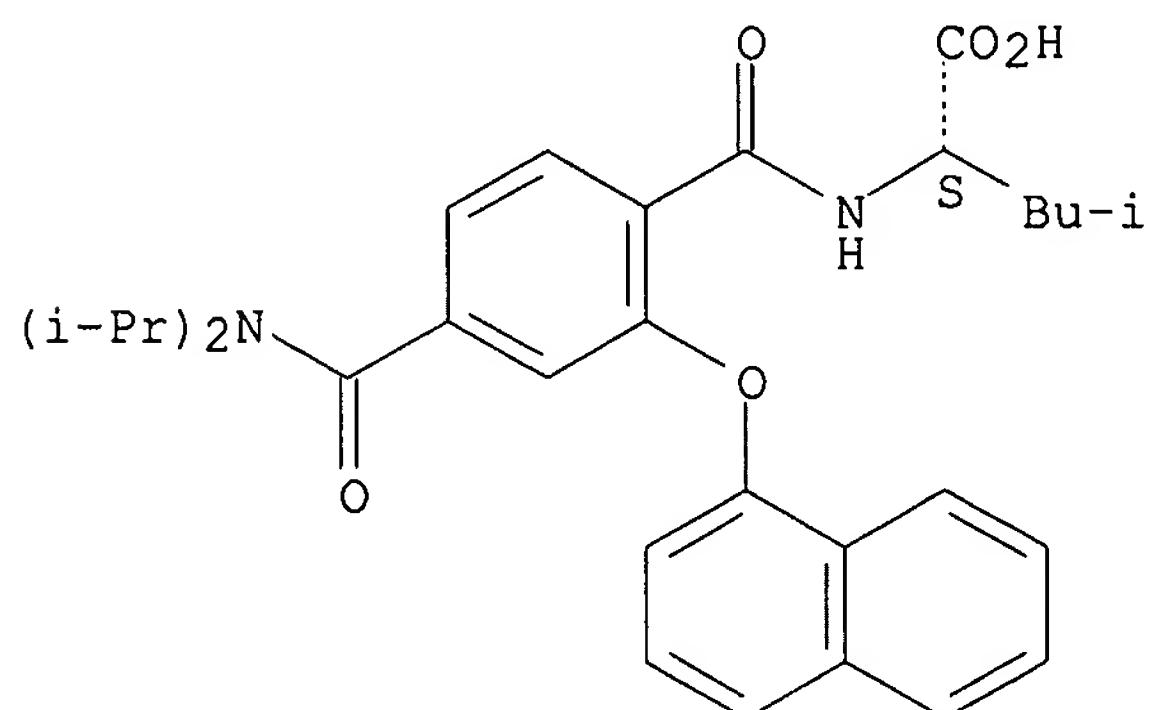
RN 681465-64-5 CAPLUS  
 CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-phenoxybenzoyl]-  
     (CA INDEX NAME)

Absolute stereochemistry.



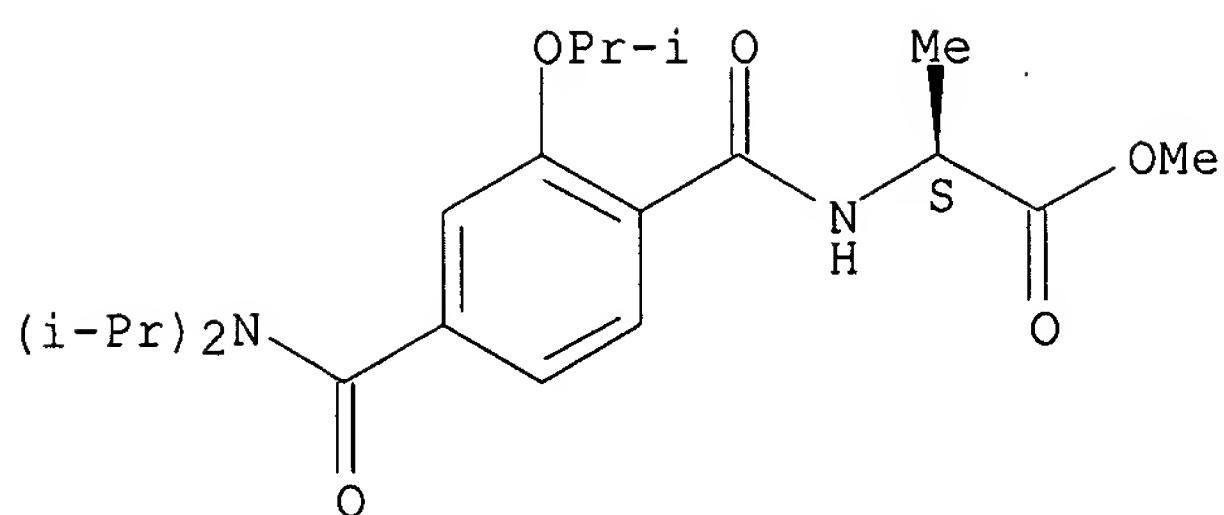
RN 681465-66-7 CAPLUS  
 CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-naphthoxy)benzoyl]-  
     (CA INDEX NAME)

Absolute stereochemistry.



RN 681465-68-9 CAPLUS  
 CN L-Alanine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester  
     (CA INDEX NAME)

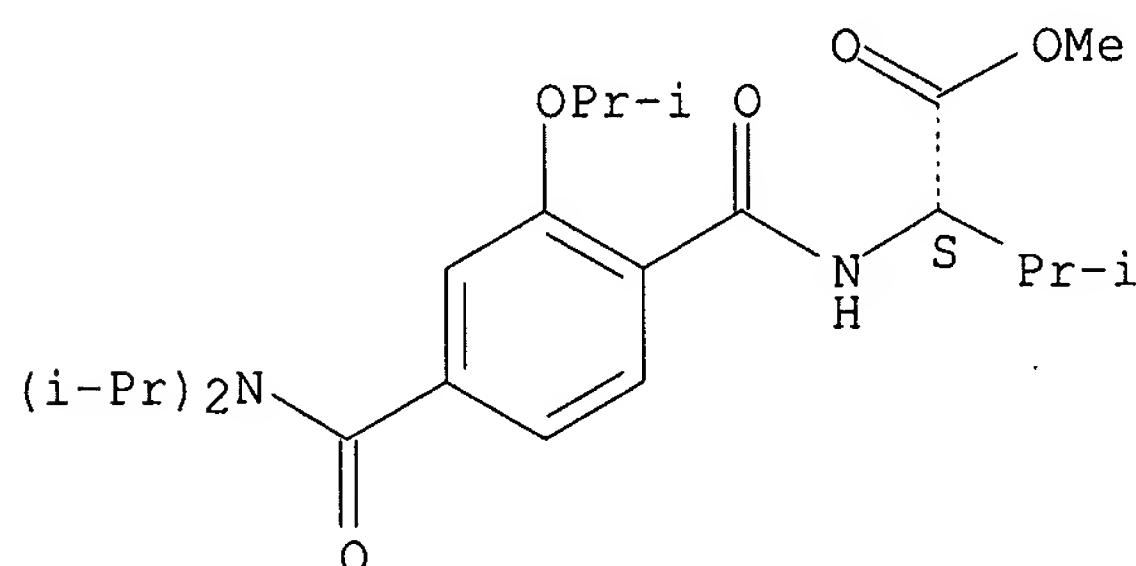
Absolute stereochemistry.



RN 681465-70-3 CAPLUS

CN L-Valine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

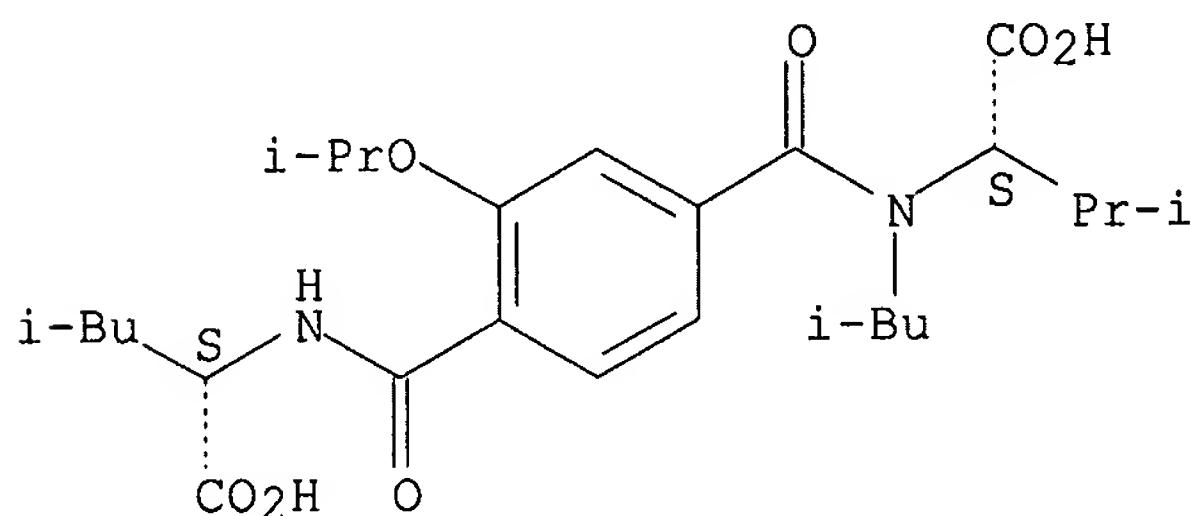
Absolute stereochemistry.



RN 681465-74-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

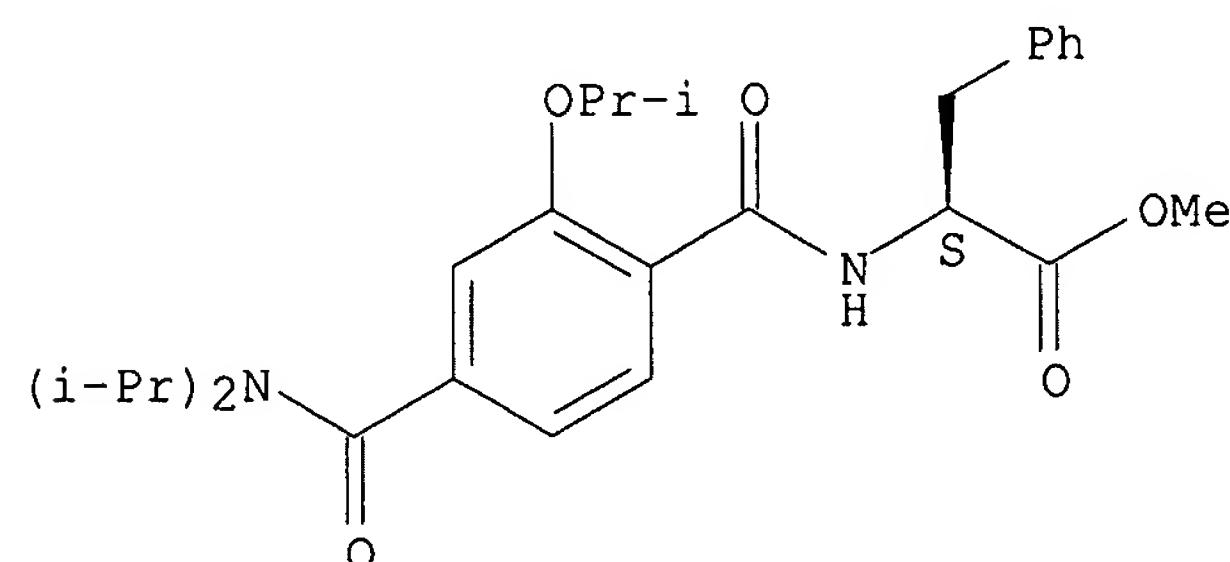
Absolute stereochemistry.



RN 852065-21-5 CAPLUS

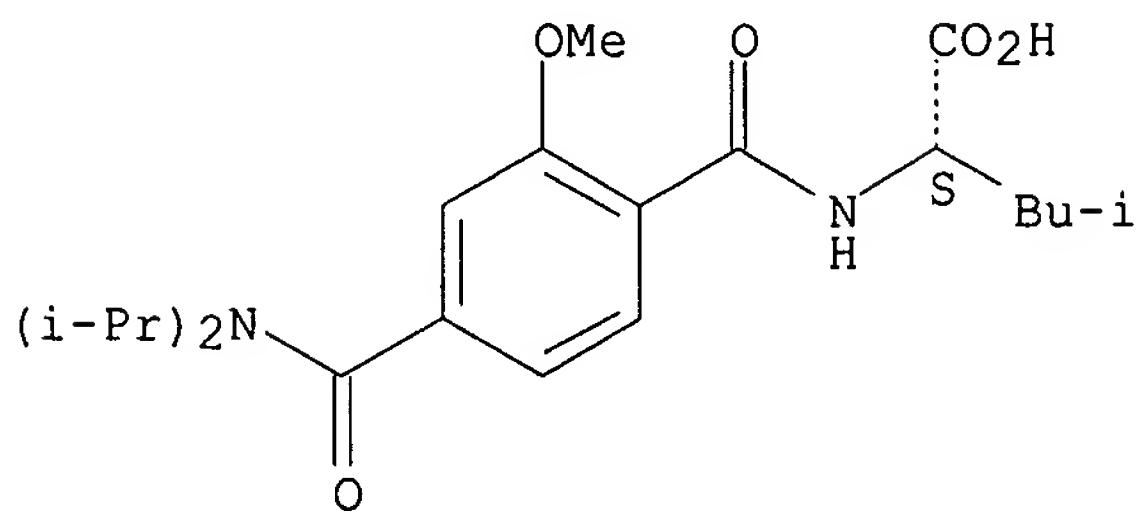
CN L-Phenylalanine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



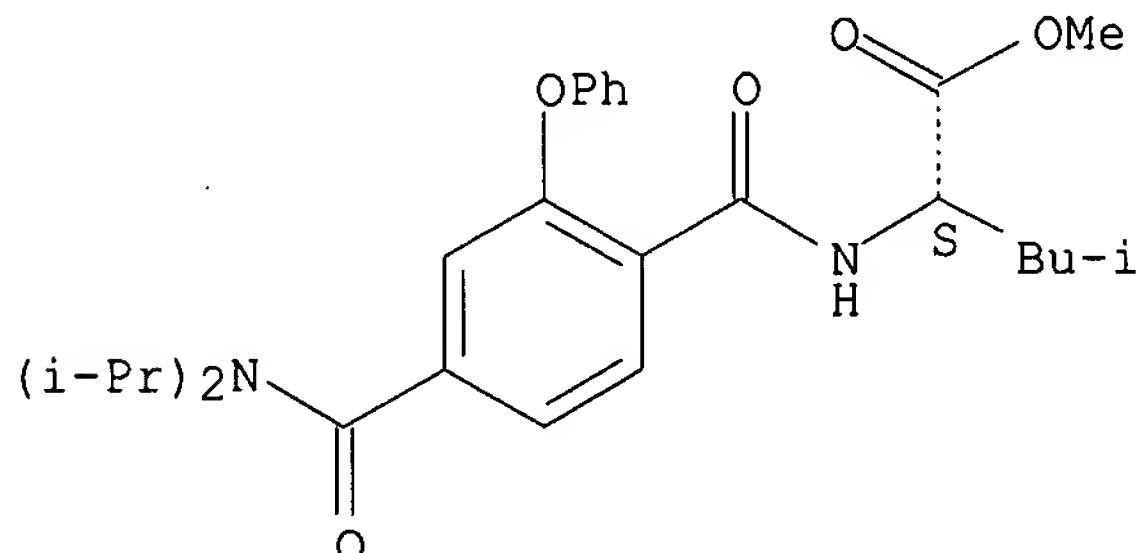
RN 852065-22-6 CAPLUS  
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-  
(CA INDEX NAME)

Absolute stereochemistry.



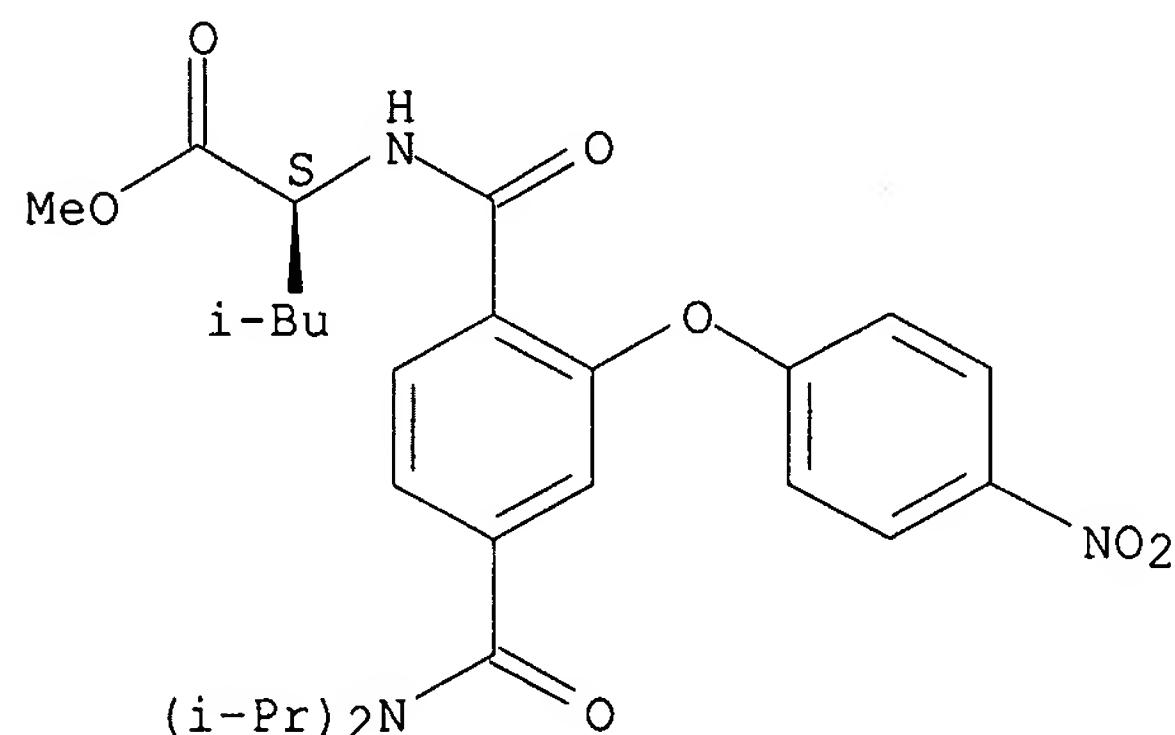
RN 852065-23-7 CAPLUS  
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-phenoxybenzoyl]-,  
methyl ester (CA INDEX NAME)

Absolute stereochemistry.



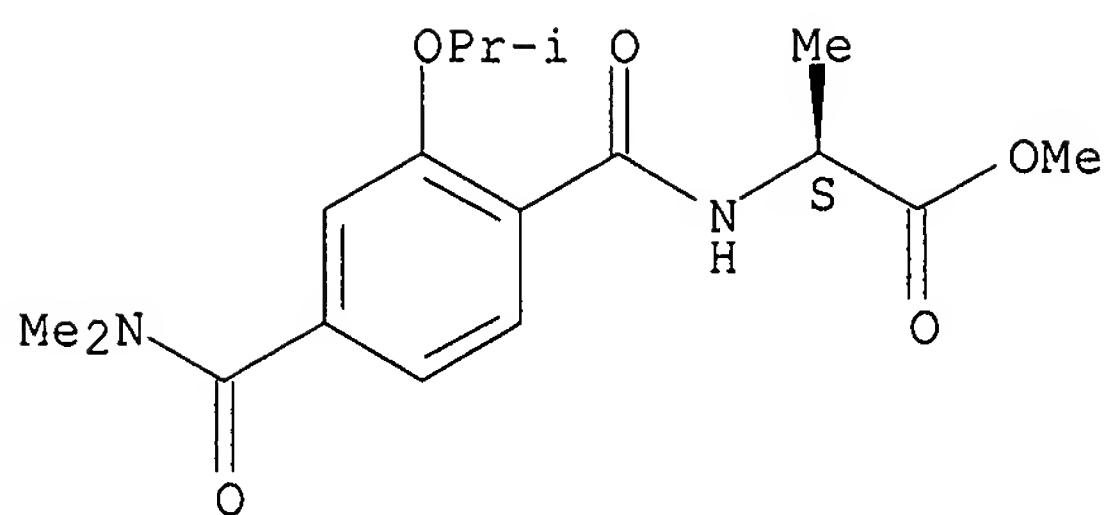
RN 852065-25-9 CAPLUS  
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(4-nitrophenoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



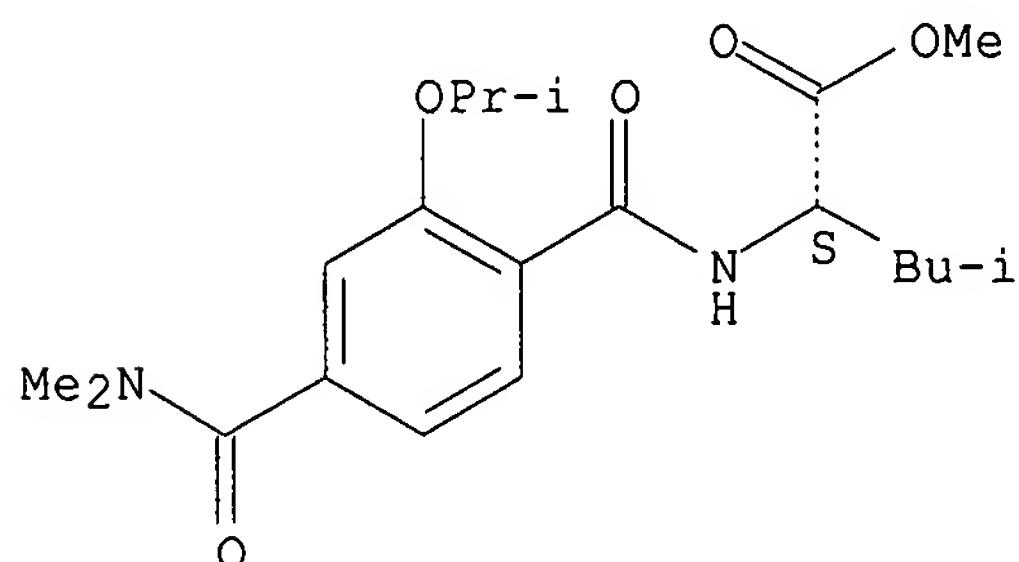
RN 852065-26-0 CAPLUS  
CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,  
methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



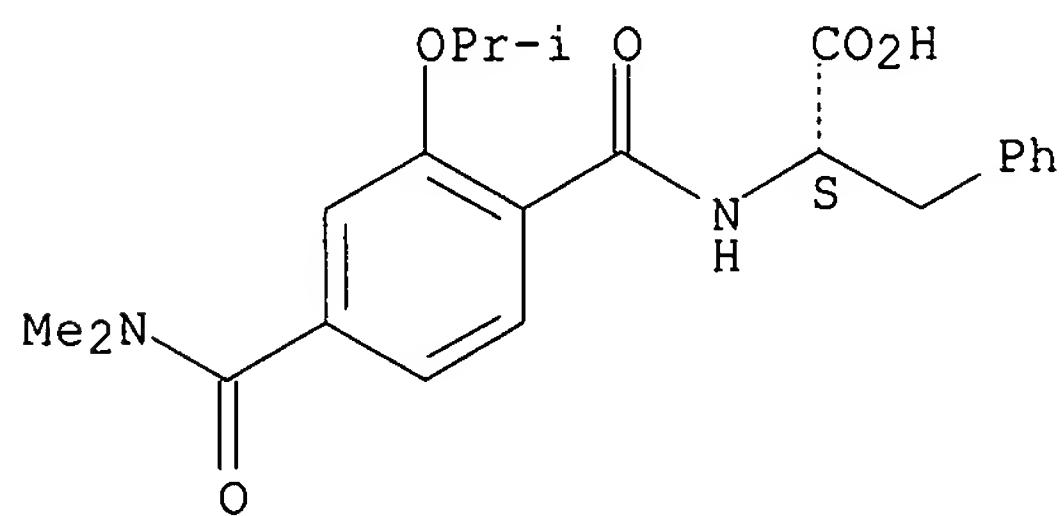
RN 852065-27-1 CAPLUS  
 CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,  
 methyl ester (CA INDEX NAME)

Absolute stereochemistry.



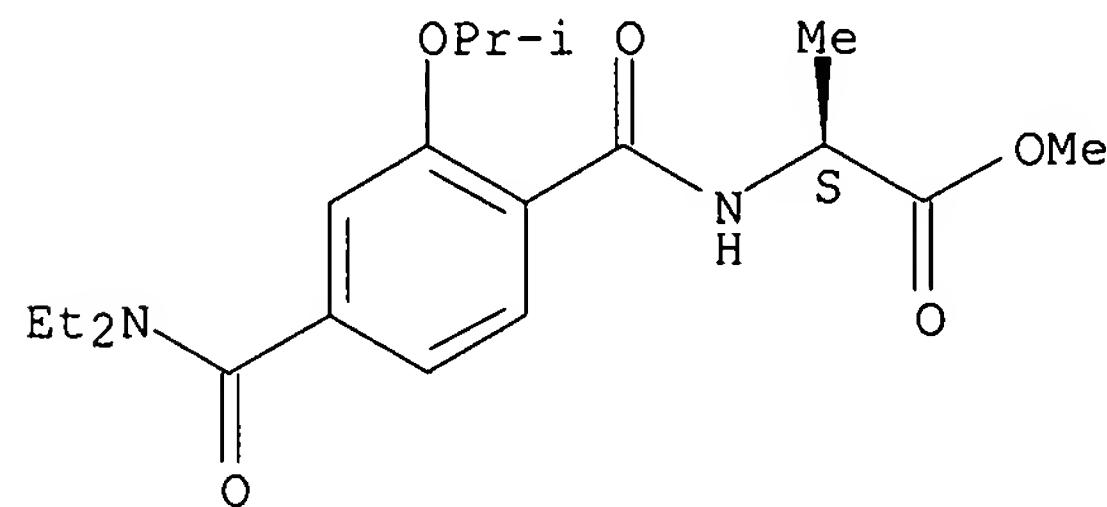
RN 852065-28-2 CAPLUS  
 CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 852065-29-3 CAPLUS  
 CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-,  
 methyl ester (CA INDEX NAME)

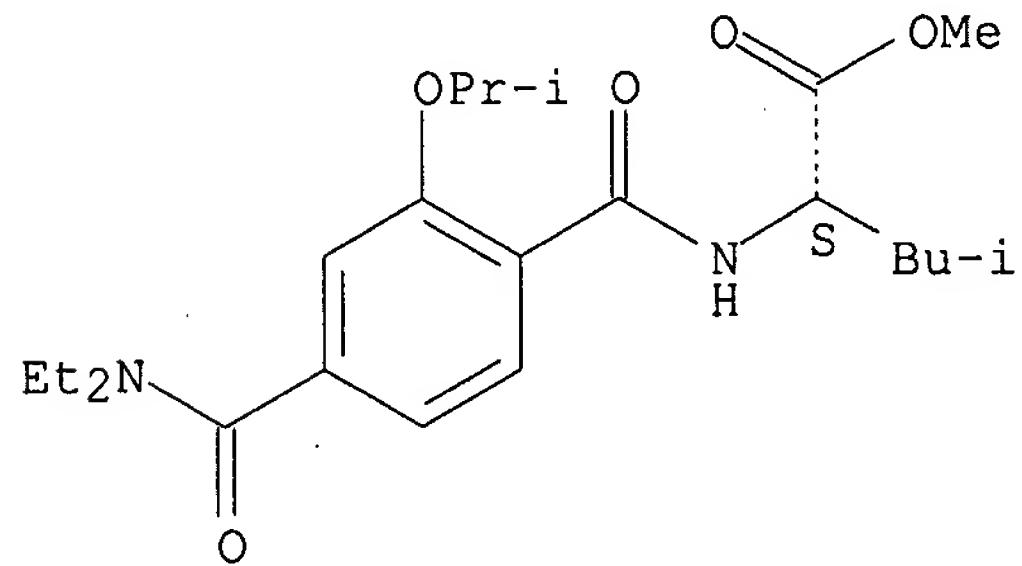
Absolute stereochemistry. Rotation (+).



RN 852065-30-6 CAPLUS

CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

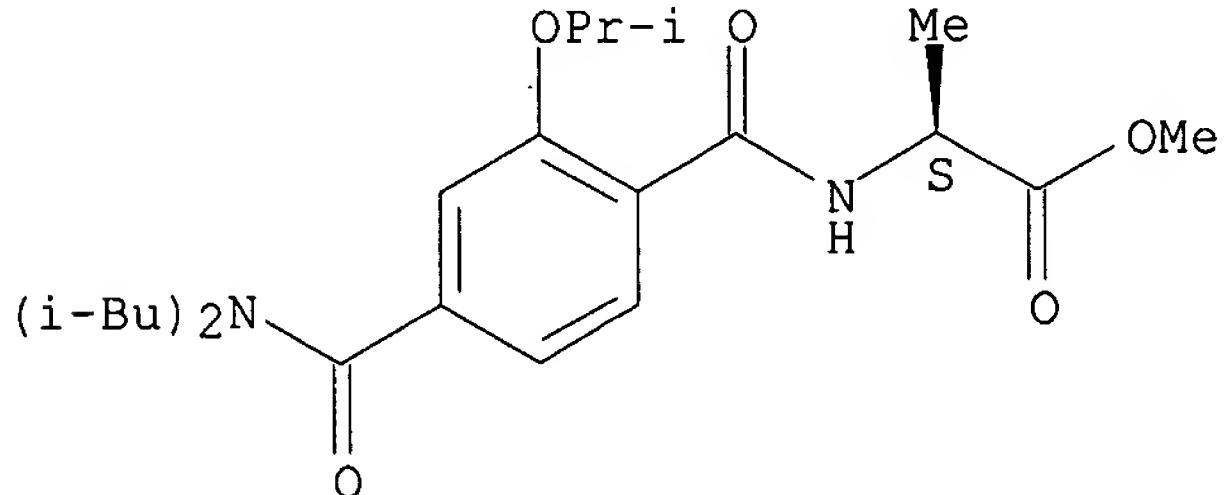
Absolute stereochemistry. Rotation (+).



RN 852065-31-7 CAPLUS

CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

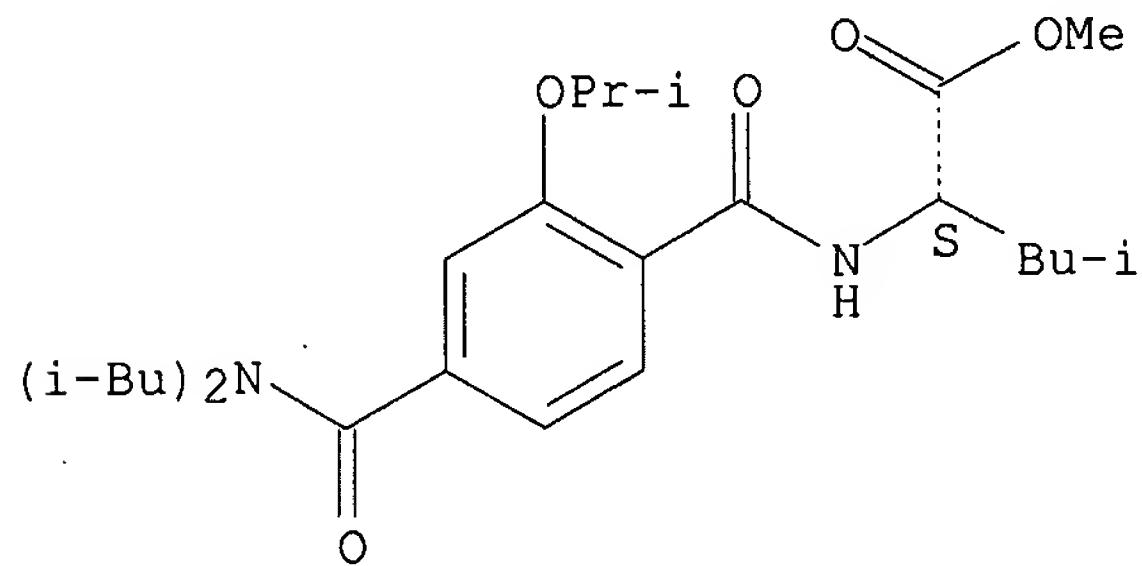
Absolute stereochemistry. Rotation (+).



RN 852065-32-8 CAPLUS

CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

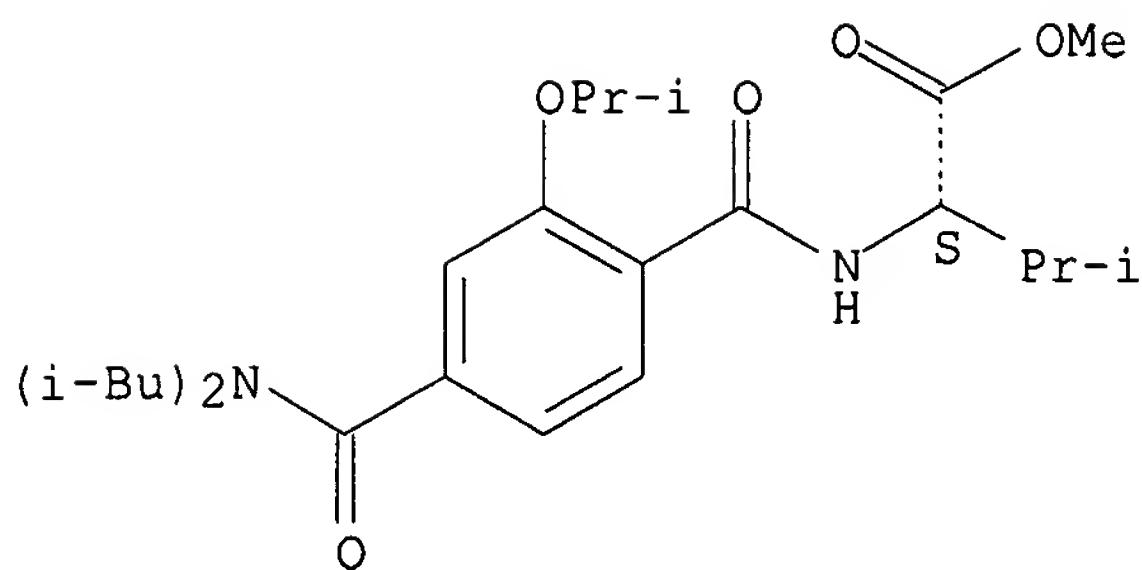
Absolute stereochemistry. Rotation (+).



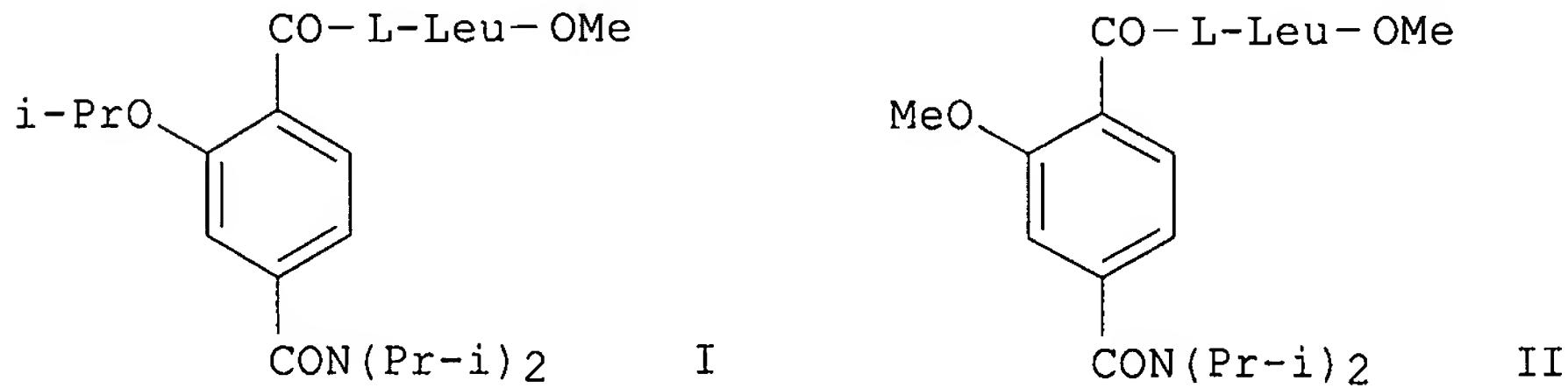
RN 852065-33-9 CAPLUS

CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 2005:267006 CAPLUS  
 DN 142:482288  
 TI Terephthalamide Derivatives as Mimetics of Helical Peptides: Disruption of the Bcl-xL/Bak Interaction  
 AU Yin, Hang; Lee, Gui-in; Sedey, Kristine A.; Rodriguez, Johanna M.; Wang, Hong-Gang; Sebti, Said M.; Hamilton, Andrew D.  
 CS Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA  
 SO Journal of the American Chemical Society (2005), 127(15), 5463-5468  
 CODEN: JACSAT; ISSN: 0002-7863  
 PB American Chemical Society  
 DT Journal  
 LA English  
 OS CASREACT 142:482288  
 GI

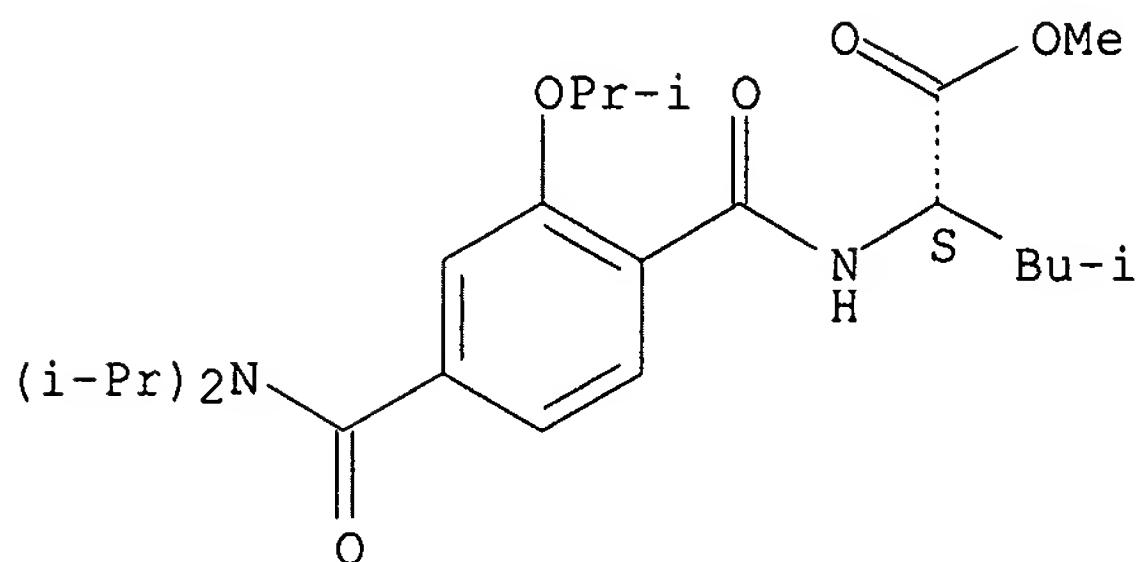


AB A series of Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, was designed to mimic the  $\alpha$ -helical region of the Bak peptide. These mols. showed favorable in-vitro activities in disrupting the Bcl-xL/Bak BH3 domain complex (terephthalamides I and II,  $K_i = 0.78 \pm 0.07$  and  $1.85 \pm 0.32 \mu\text{M}$ , resp.). Extensive structure-affinity studies demonstrated a correlation between the ability of terephthalamide derivs. to disrupt Bcl-xL/Bak complex formation and the size of variable side chains on these mols. Treatment of human HEK293 cells with the terephthalamide derivative 26 resulted in disruption of the Bcl-xL/Bax interaction in whole cells with an IC<sub>50</sub> of  $35.0 \mu\text{M}$ . Computational docking simulations and NMR expts. suggested that the binding cleft for the BH3 domain of the Bak peptide on the surface of Bcl-xL is the target area for these synthetic inhibitors.

IT 681465-54-3P  
 RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-54-3 CAPLUS  
 CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-58-7P 681465-60-1P  
681465-62-3P 681465-64-5P 681465-68-9P  
681465-70-3P 681465-74-7P 852065-21-5P  
852065-22-6P 852065-23-7P 852065-24-8P  
852065-25-9P 852065-26-0P 852065-27-1P  
852065-28-2P 852065-29-3P 852065-30-6P  
852065-31-7P 852065-32-8P 852065-33-9P

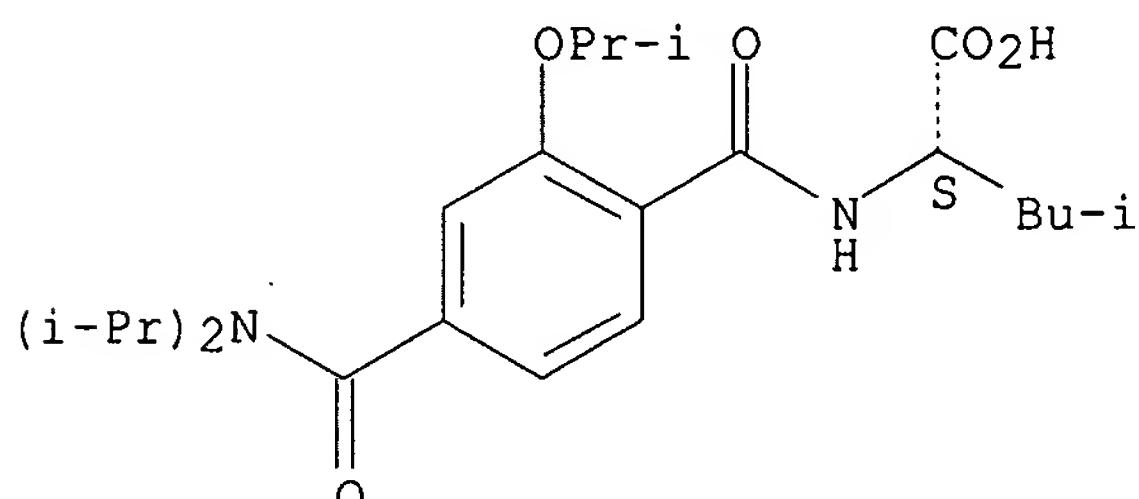
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation of terephthalamide derivs. as helical peptidomimetics and their evaluation as antagonists of Bcl-x/Bak protein interaction)

RN 681465-56-5 CAPLUS

CN L-Leucine, N-[4-[[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

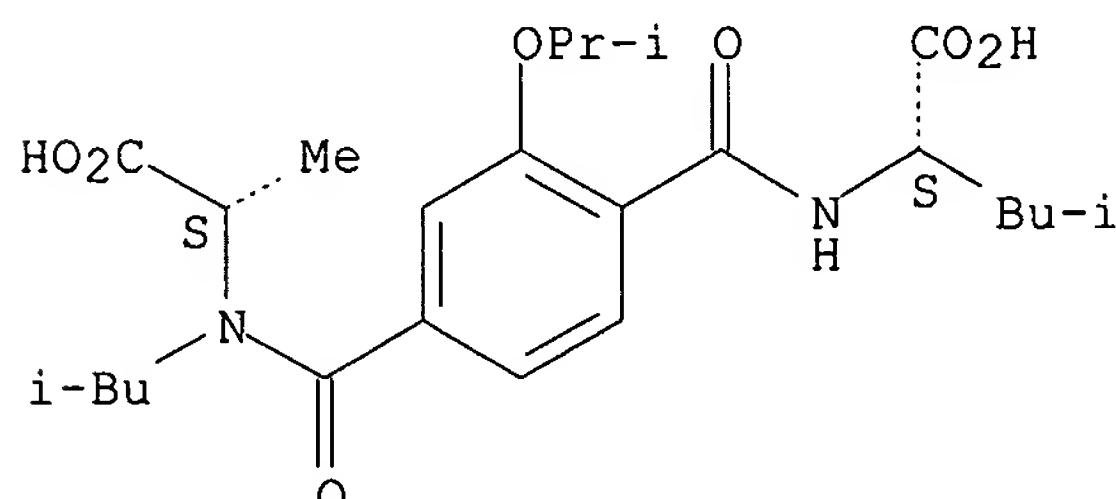
Absolute stereochemistry.



RN 681465-58-7 CAPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

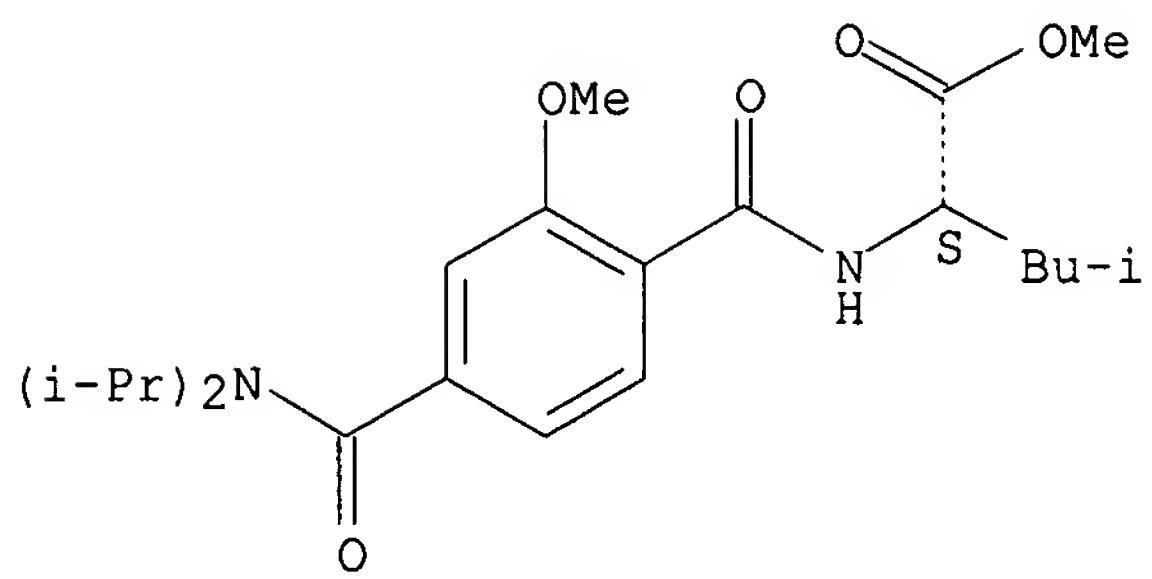
Absolute stereochemistry. Rotation (-).



RN 681465-60-1 CAPLUS

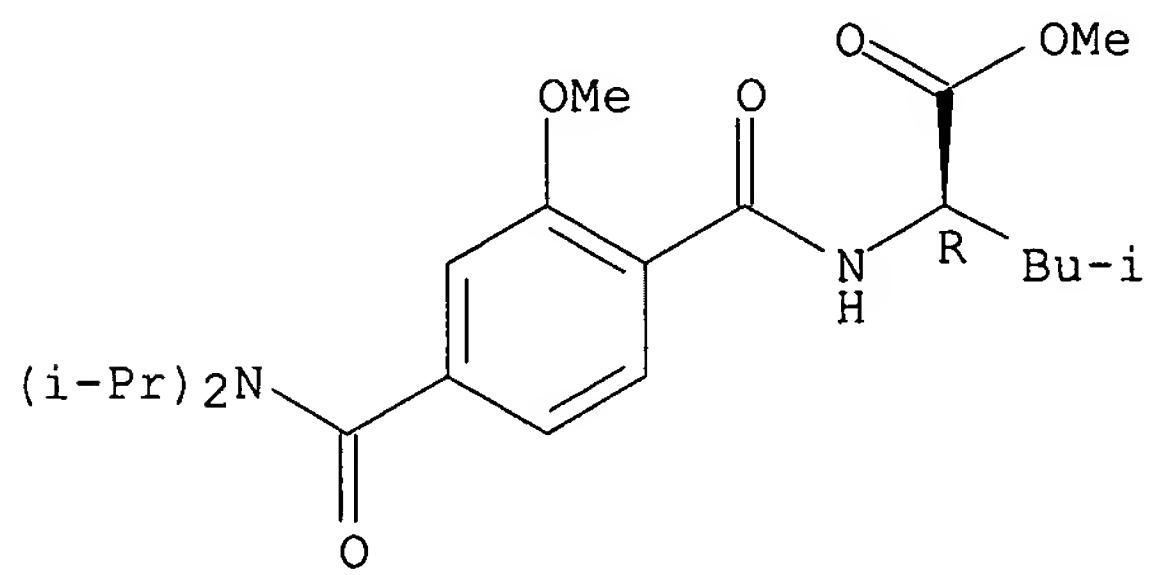
CN L-Leucine, N-[4-[[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



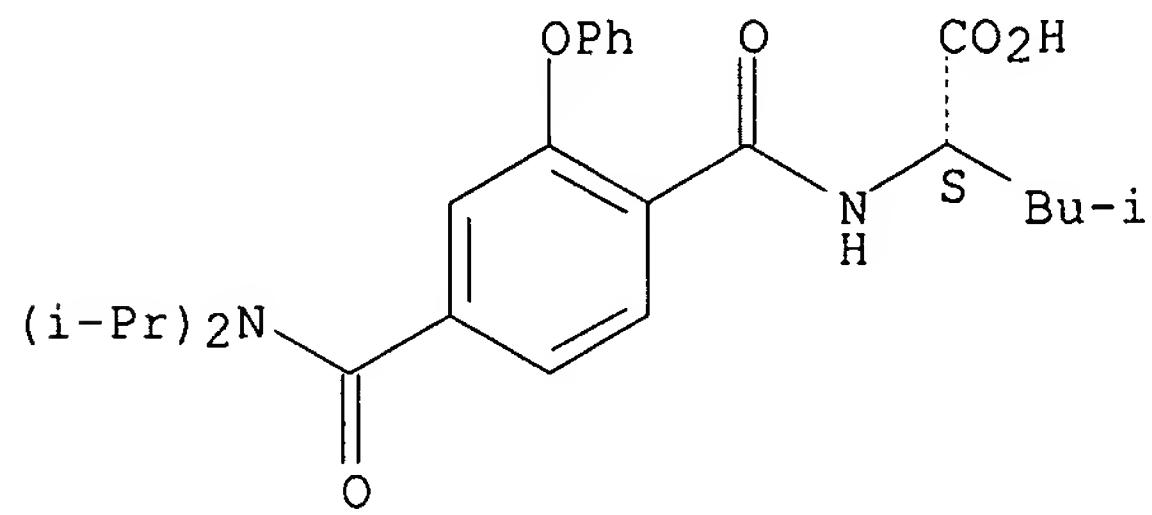
RN 681465-62-3 CAPLUS  
CN D-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



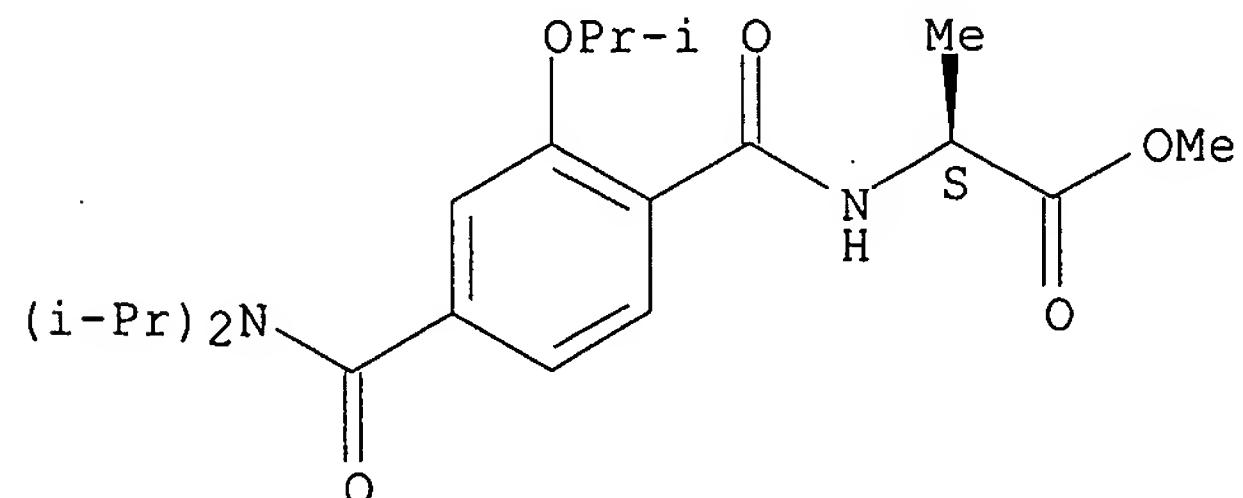
RN 681465-64-5 CAPLUS  
CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-phenoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



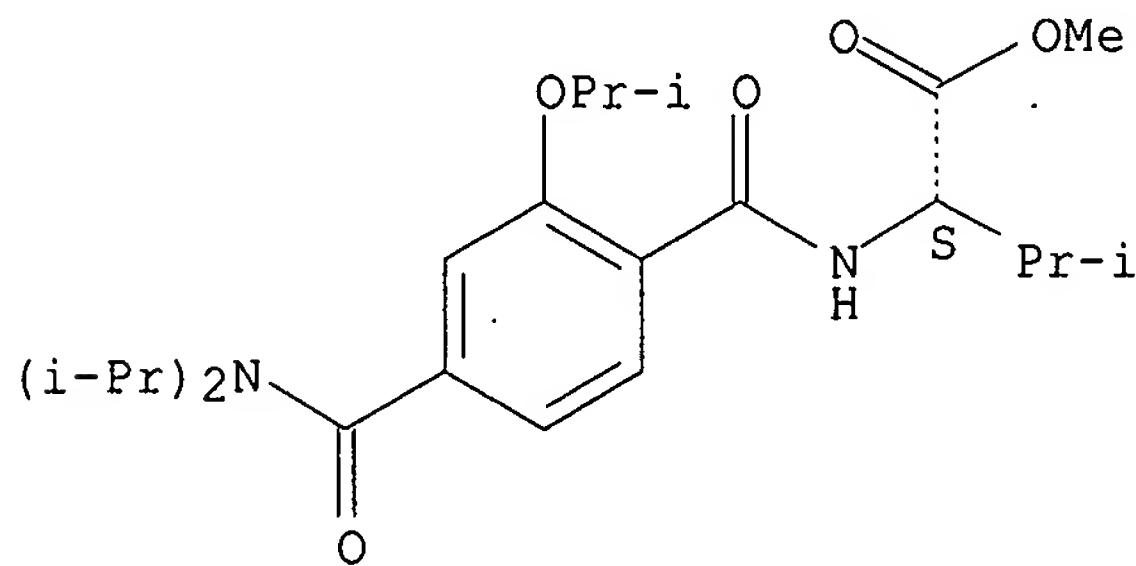
RN 681465-68-9 CAPLUS  
CN L-Alanine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



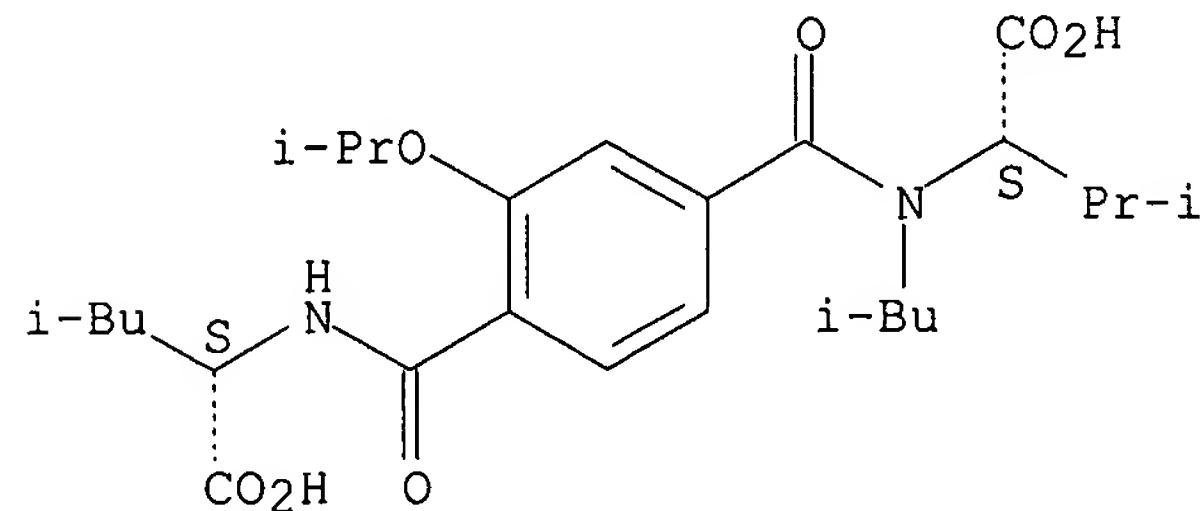
RN 681465-70-3 CAPLUS  
CN L-Valine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



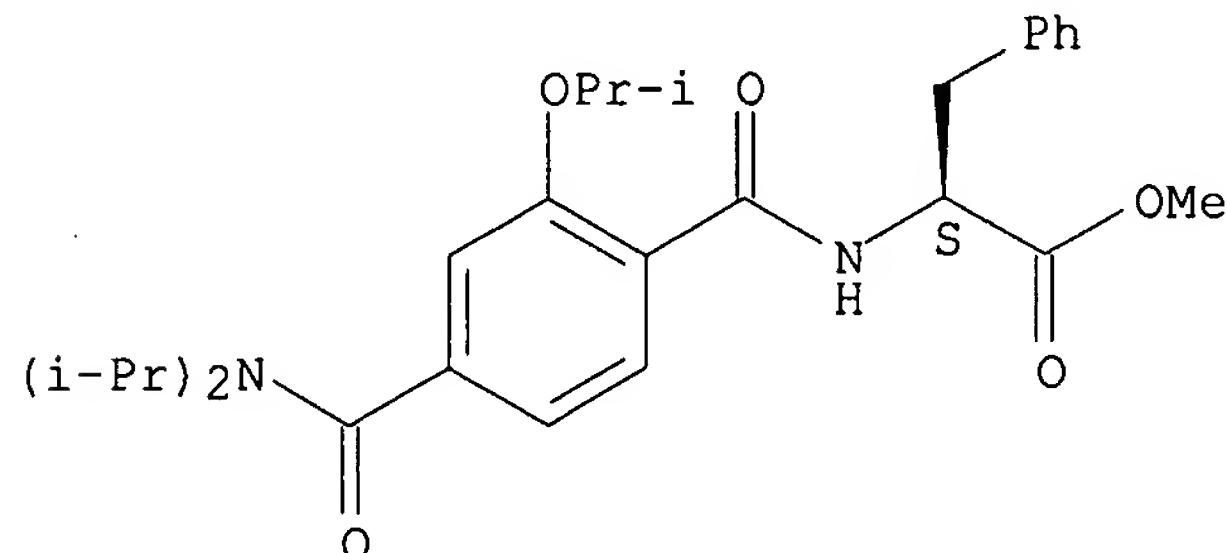
RN 681465-74-7 CAPLUS  
CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



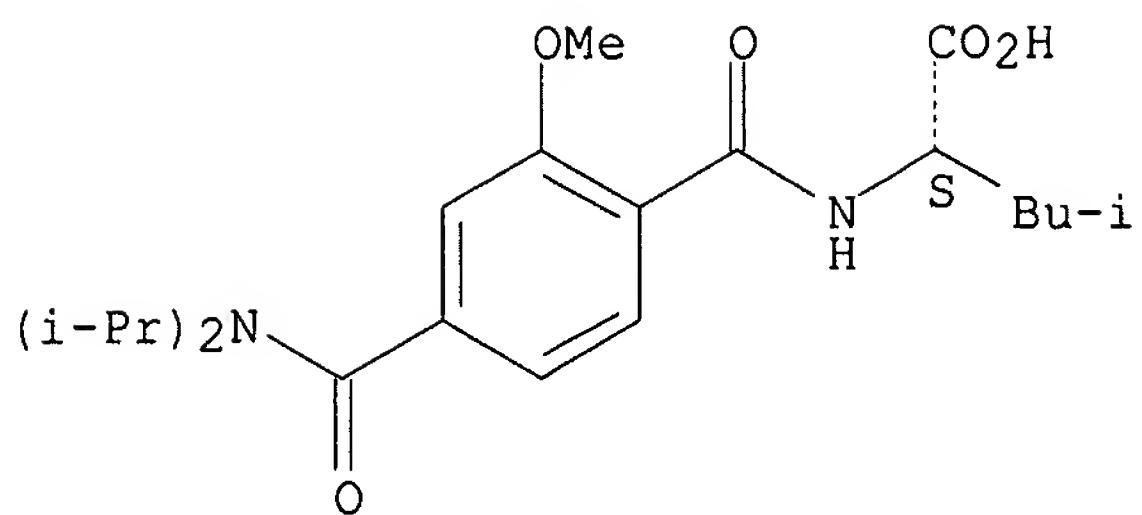
RN 852065-21-5 CAPLUS  
CN L-Phenylalanine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



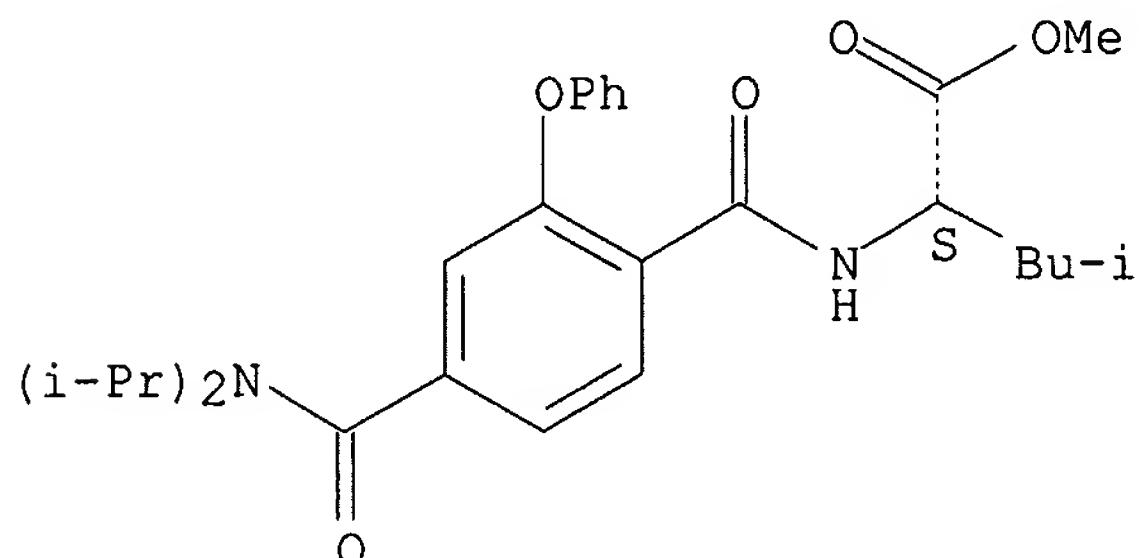
RN 852065-22-6 CAPLUS  
CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-methoxybenzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



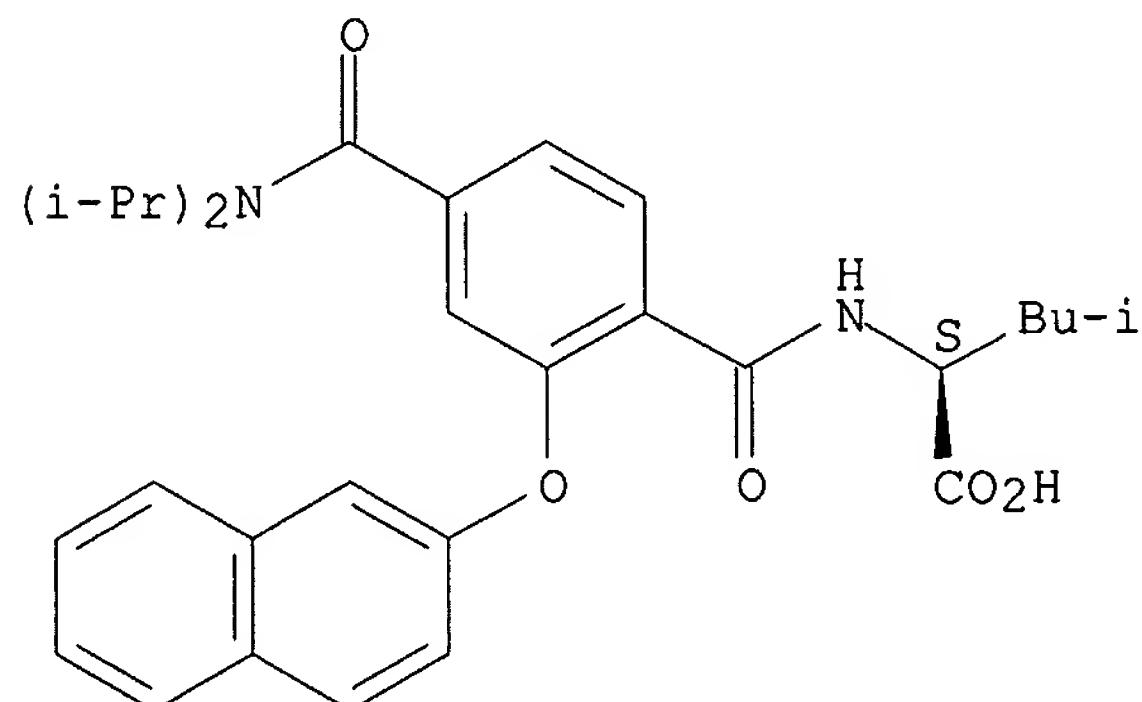
RN 852065-23-7 CAPLUS  
 CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-phenoxybenzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry.



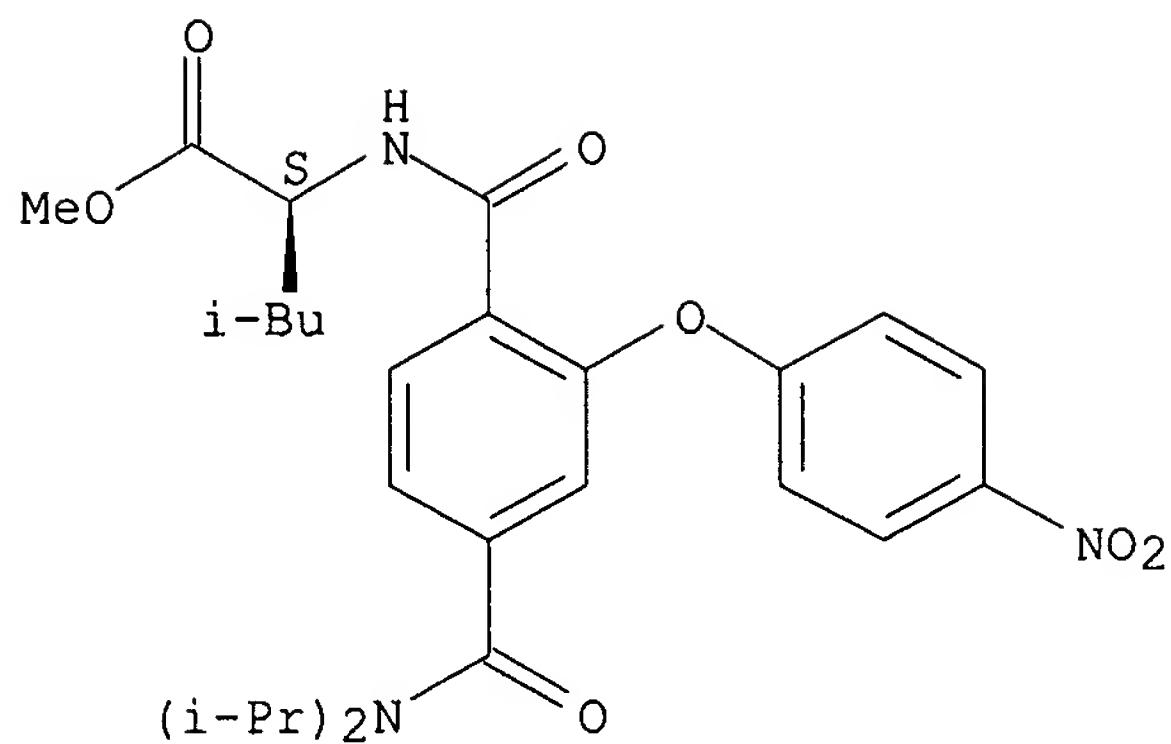
RN 852065-24-8 CAPLUS  
 CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(2-naphthalenyl)benzoyl]- (CA INDEX NAME)

Absolute stereochemistry.



RN 852065-25-9 CAPLUS  
 CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(4-nitrophenoxy)benzoyl]-, methyl ester (CA INDEX NAME)

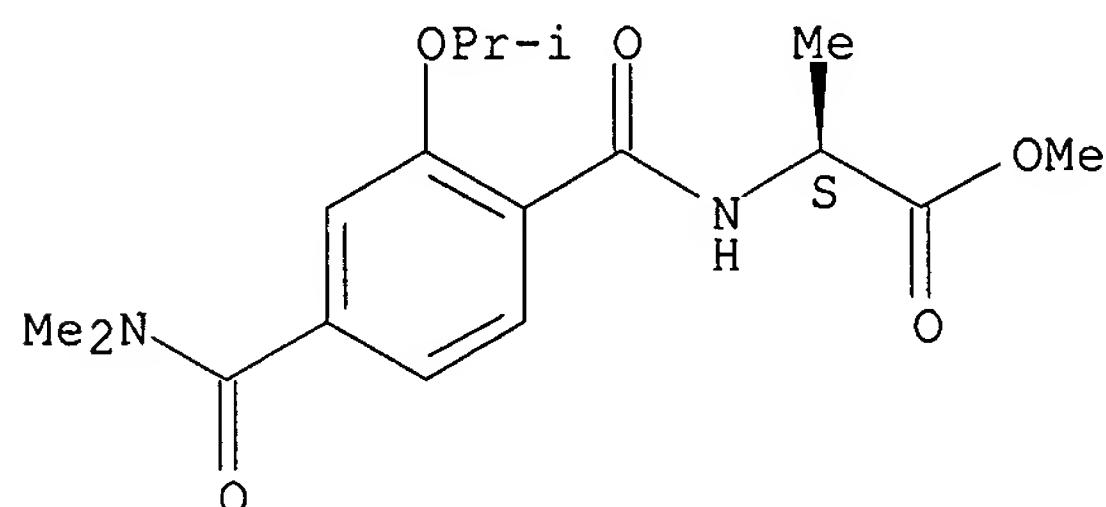
Absolute stereochemistry.



RN 852065-26-0 CAPLUS

CN L-Alanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

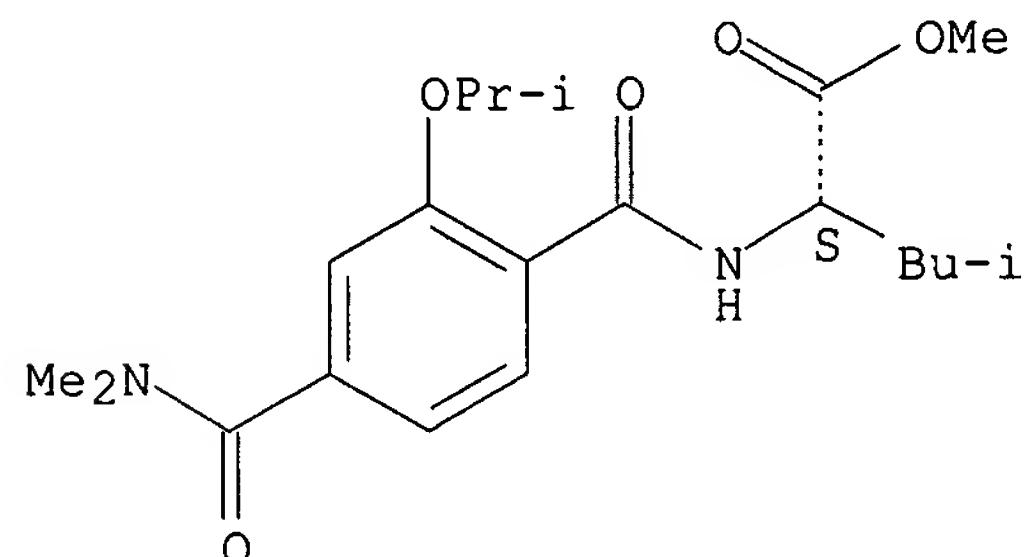
Absolute stereochemistry. Rotation (+).



RN 852065-27-1 CAPLUS

CN L-Leucine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

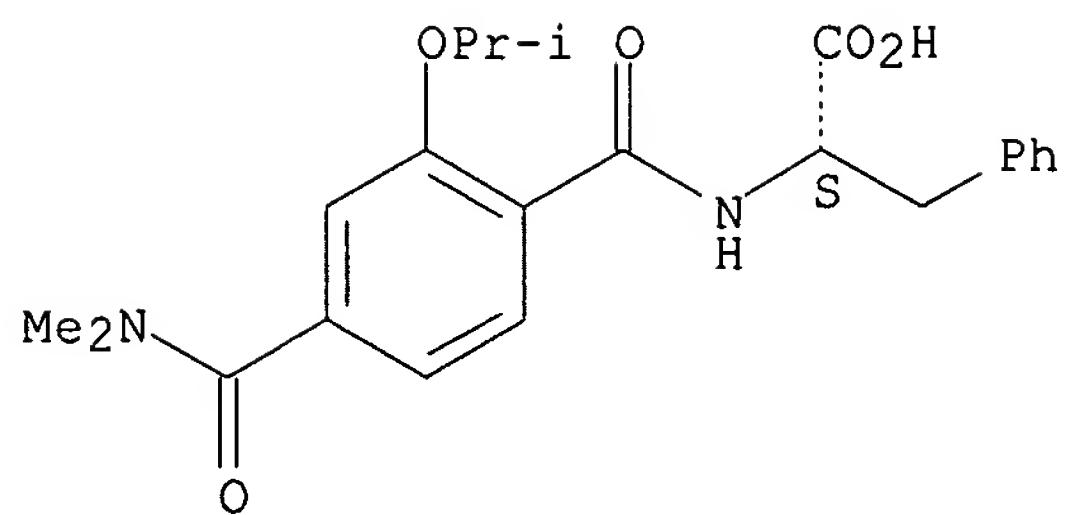
Absolute stereochemistry.



RN 852065-28-2 CAPLUS

CN L-Phenylalanine, N-[4-[(dimethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

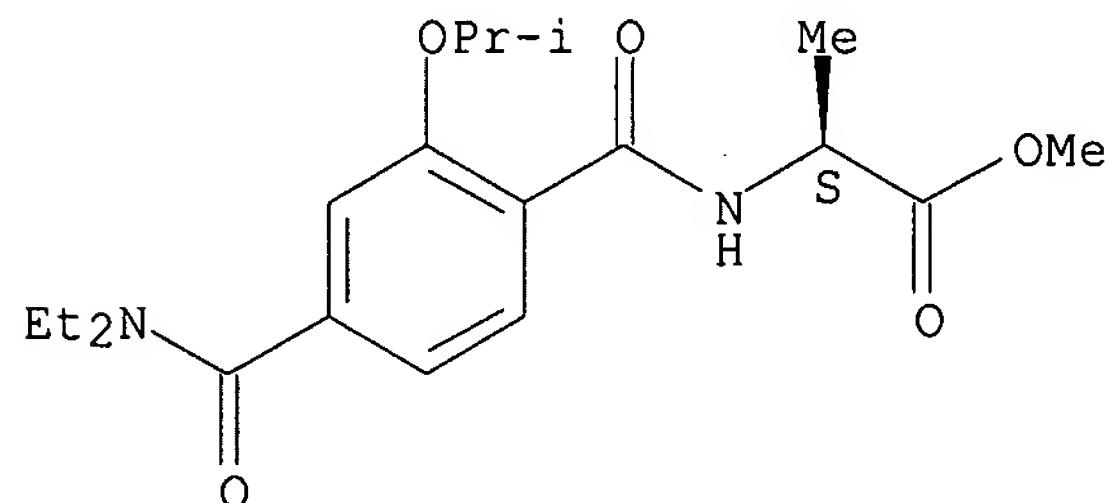
Absolute stereochemistry. Rotation (+).



RN 852065-29-3 CAPLUS

CN L-Alanine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

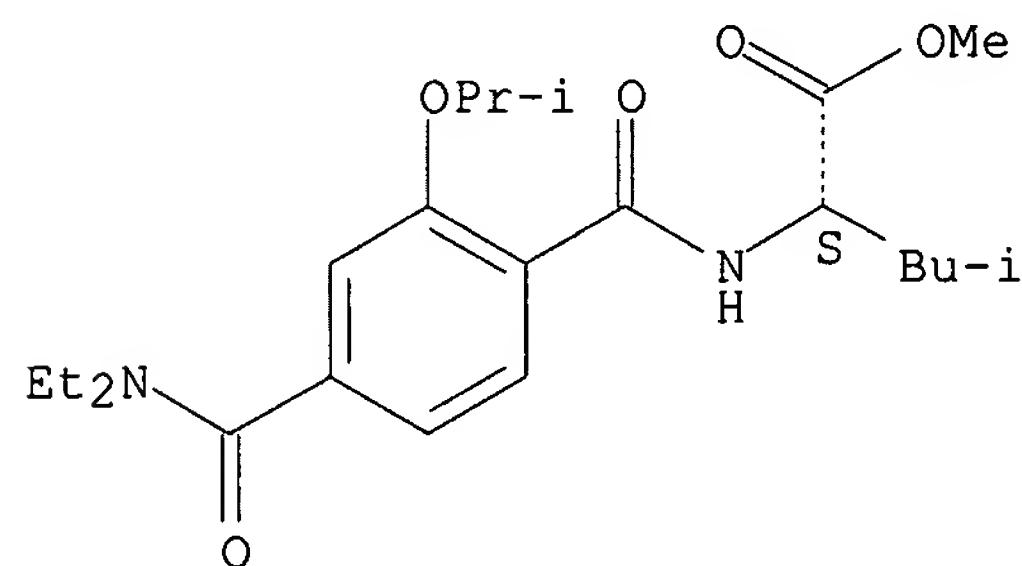
Absolute stereochemistry. Rotation (+).



RN 852065-30-6 CAPLUS

CN L-Leucine, N-[4-[(diethylamino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

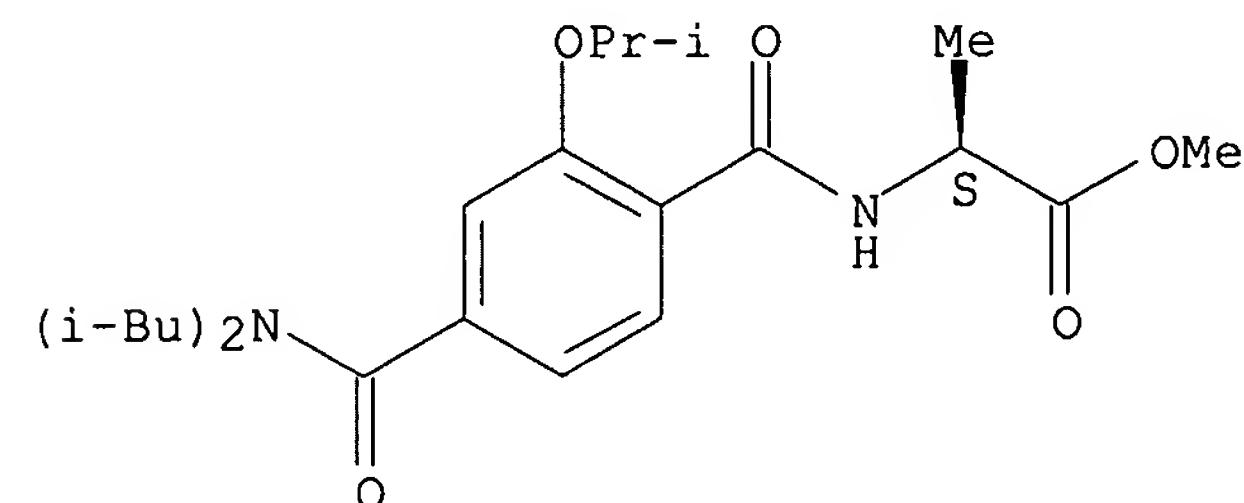
Absolute stereochemistry. Rotation (+).



RN 852065-31-7 CAPLUS

CN L-Alanine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

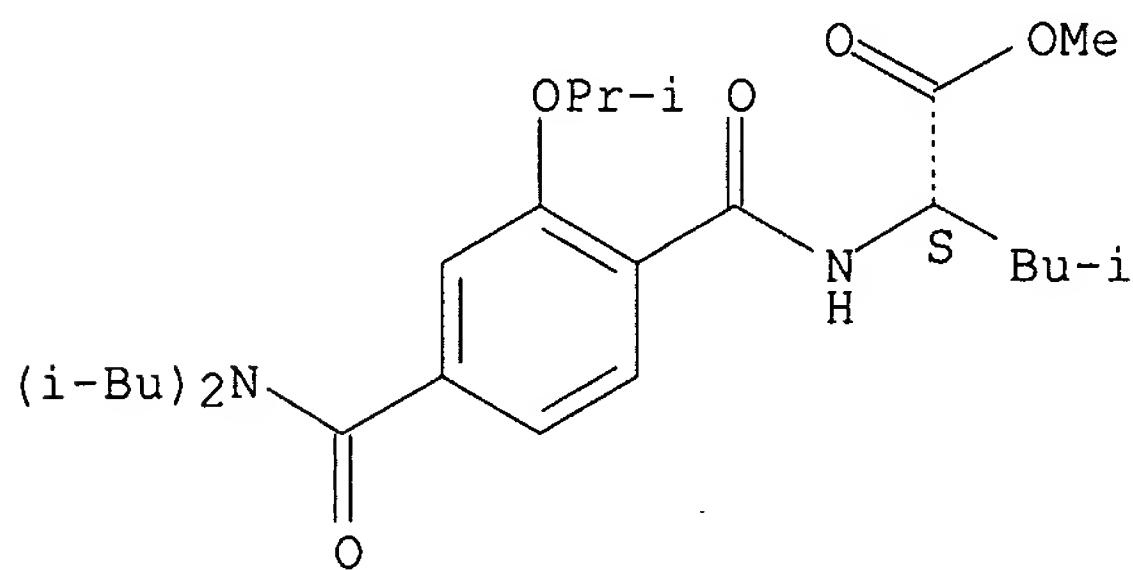
Absolute stereochemistry. Rotation (+).



RN 852065-32-8 CAPLUS

CN L-Leucine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

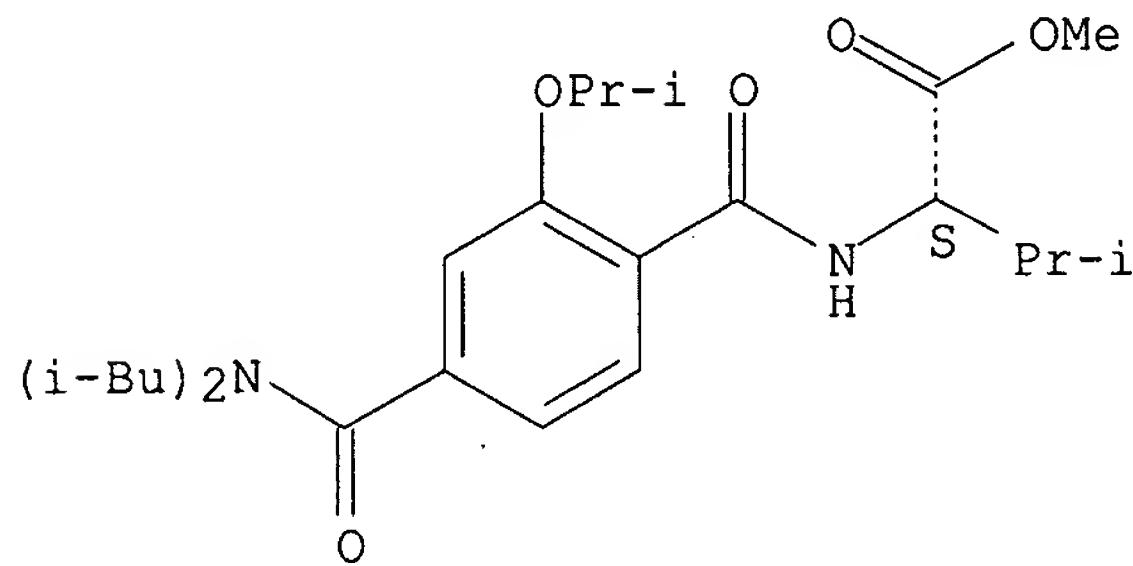
Absolute stereochemistry. Rotation (+).



RN 852065-33-9 CAPLUS

CN L-Valine, N-[4-[[bis(2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

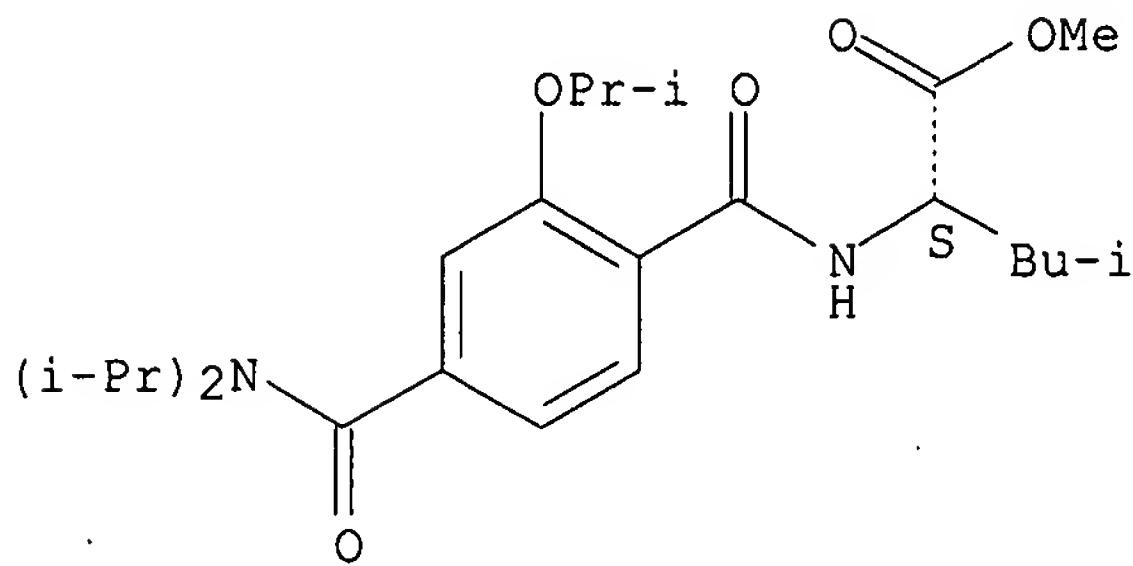
Absolute stereochemistry. Rotation (+).



RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN  
AN 2004:189140 CAPLUS  
DN 140:350050  
TI Terephthalamide derivatives as mimetics of the helical region of Bak peptide target Bcl-xL protein  
AU Yin, Hang; Hamilton, Andrew D.  
CS Department of Chemistry, Yale University, New Haven, CT, 06511, USA  
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(6), 1375-1379  
CODEN: BMCLE8; ISSN: 0960-894X  
PB Elsevier Science B.V.  
DT Journal  
LA English  
OS CASREACT 140:350050  
AB A group of novel Bcl-xL/Bak antagonists, based on a terephthalamide scaffold, were designed to mimic the  $\alpha$ -helical region of the Bak peptide. Good in vitro inhibition potencies in disrupting the Bak/Bcl-xL complex have been observed (terephthalamide 4,  $K_i=0.78\pm0.07 \mu M$ ).  
IT 681465-54-3P  
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)  
RN 681465-54-3 CAPLUS  
CN L-Leucine, N-[4-[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-56-5P 681465-58-7P

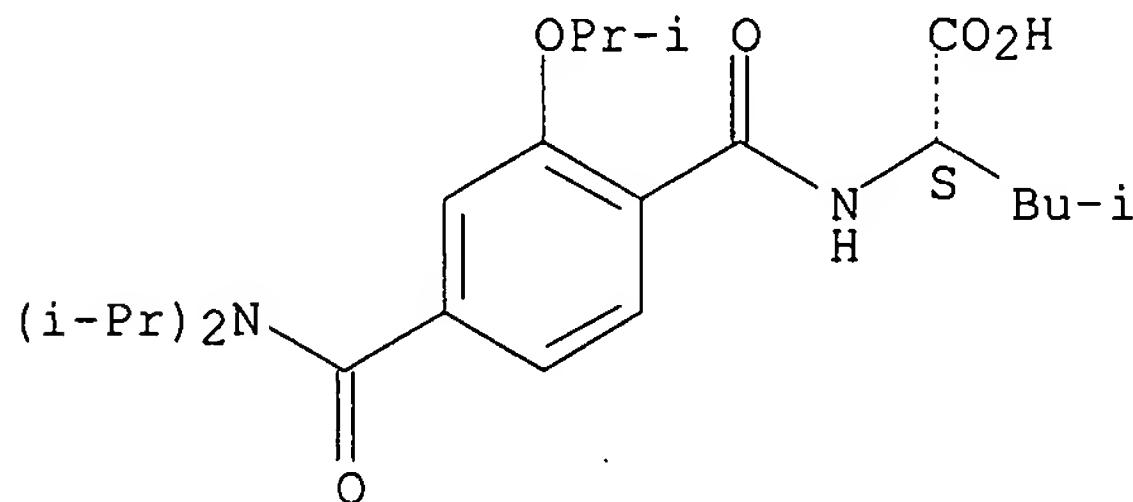
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-56-5 CAPPLUS

CN L-Leucine, N-[4-[[[bis(1-methylethyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (CA INDEX NAME)

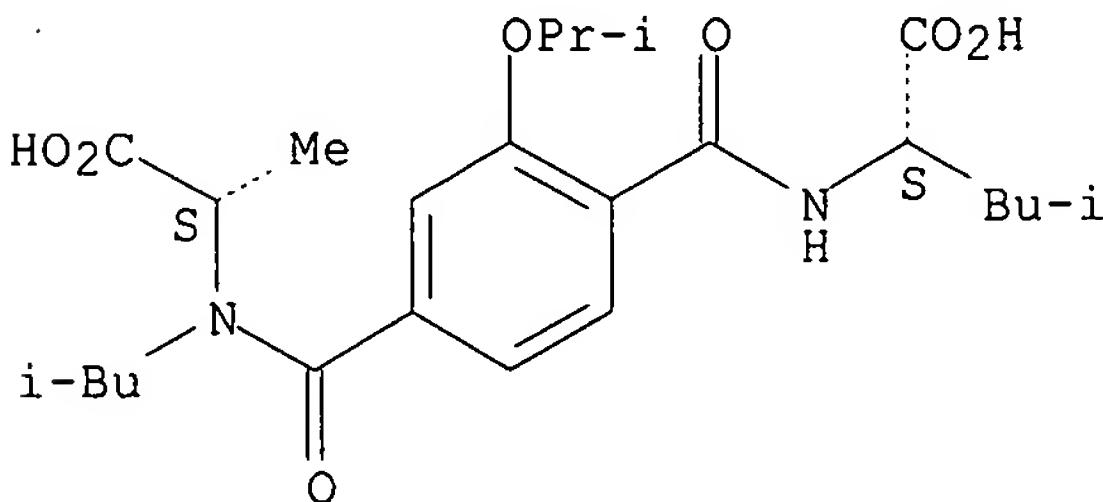
Absolute stereochemistry.



RN 681465-58-7 CAPPLUS

CN L-Leucine, N-[4-[[[(1S)-1-carboxyethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 681465-60-1 681465-62-3 681465-64-5

681465-66-7 681465-68-9 681465-70-3

681465-72-5 681465-74-7

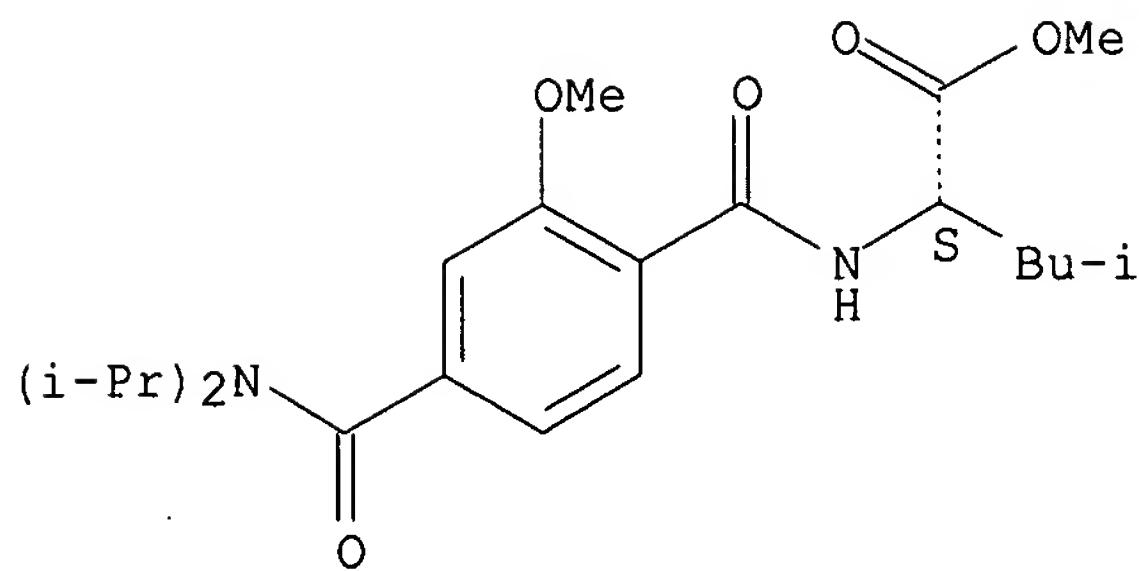
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(terephthalamide derivs. as novel Bcl-xL/Bak antagonists)

RN 681465-60-1 CAPPLUS

CN L-Leucine, N-[4-[[[bis(1-methylethyl)amino]carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

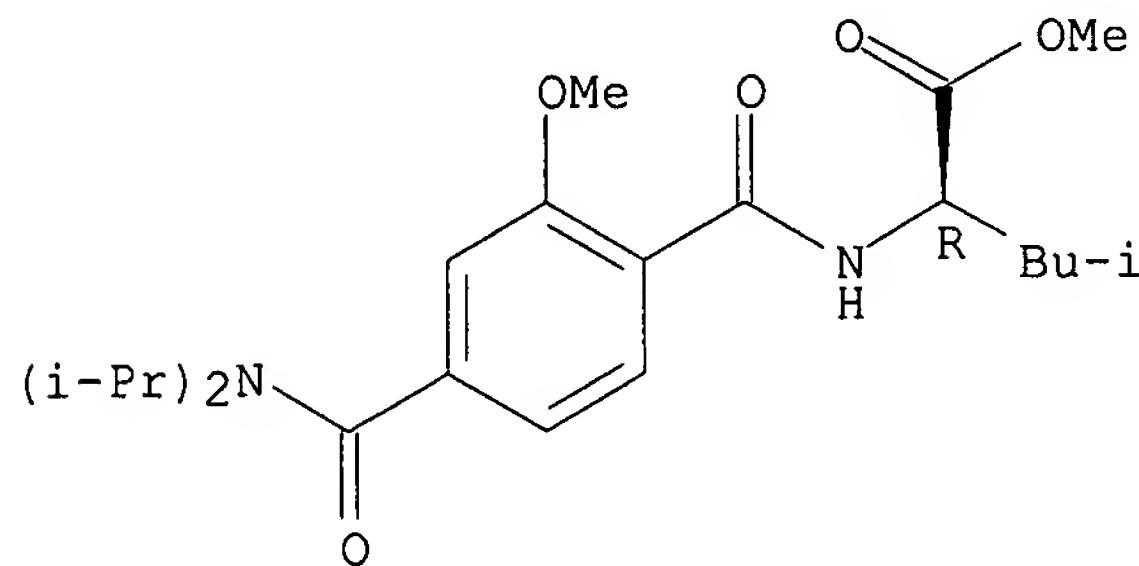
Absolute stereochemistry. Rotation (-).



RN 681465-62-3 CAPLUS

CN D-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-methoxybenzoyl]-, methyl ester (CA INDEX NAME)

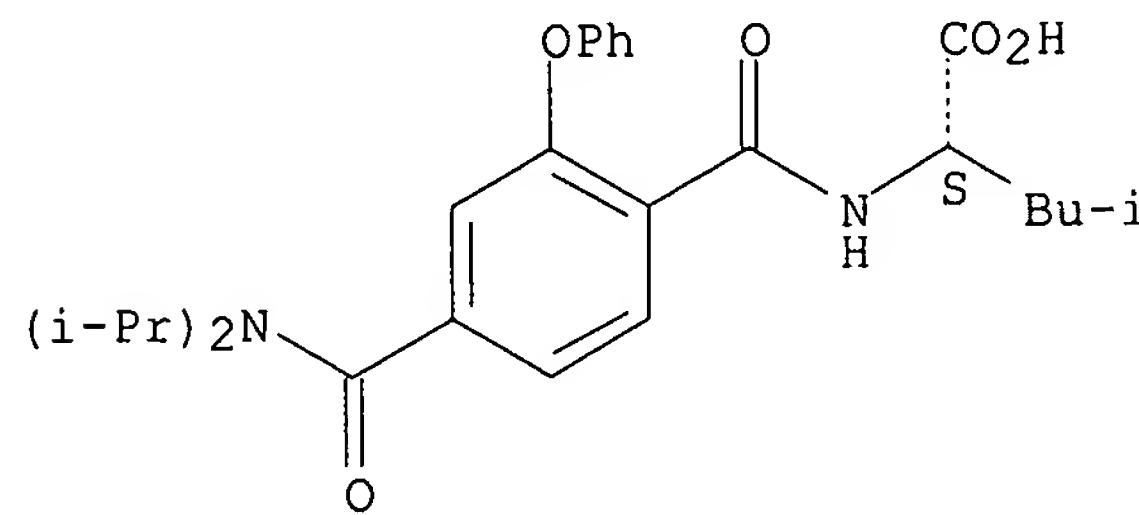
Absolute stereochemistry.



RN 681465-64-5 CAPLUS

CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-phenoxybenzoyl]- (CA INDEX NAME)

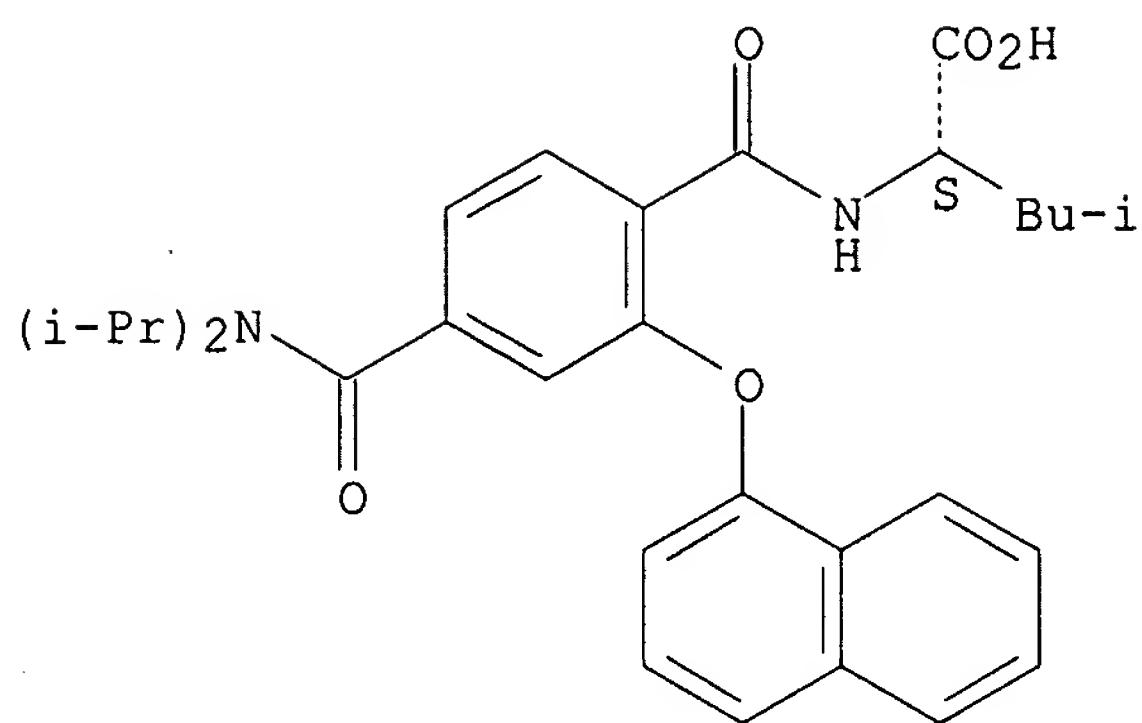
Absolute stereochemistry.



RN 681465-66-7 CAPLUS

CN L-Leucine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-naphthalenyl)benzoyl]- (CA INDEX NAME)

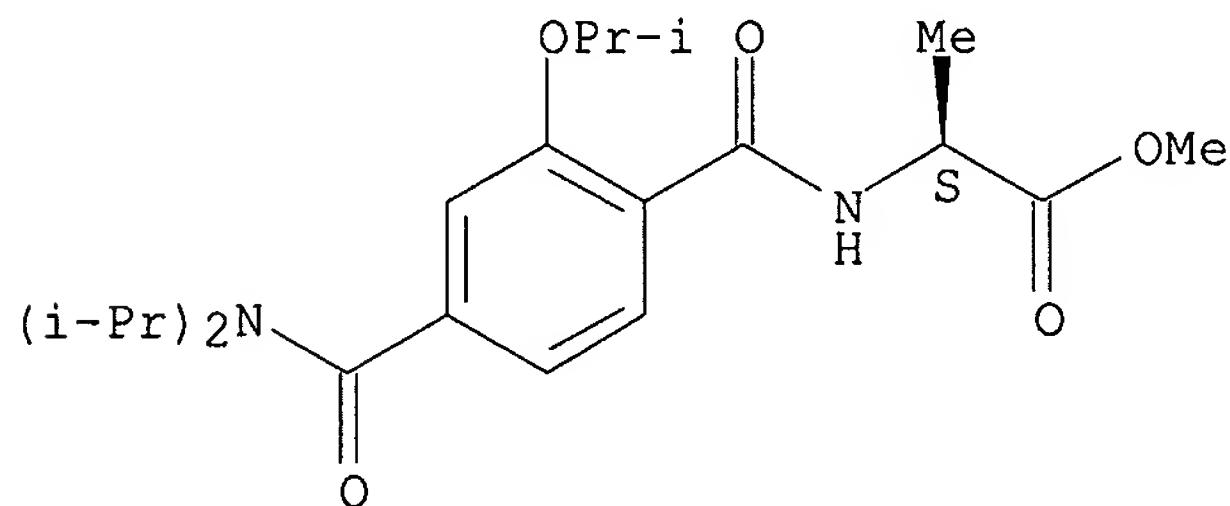
Absolute stereochemistry.



RN 681465-68-9 CAPLUS

CN L-Alanine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

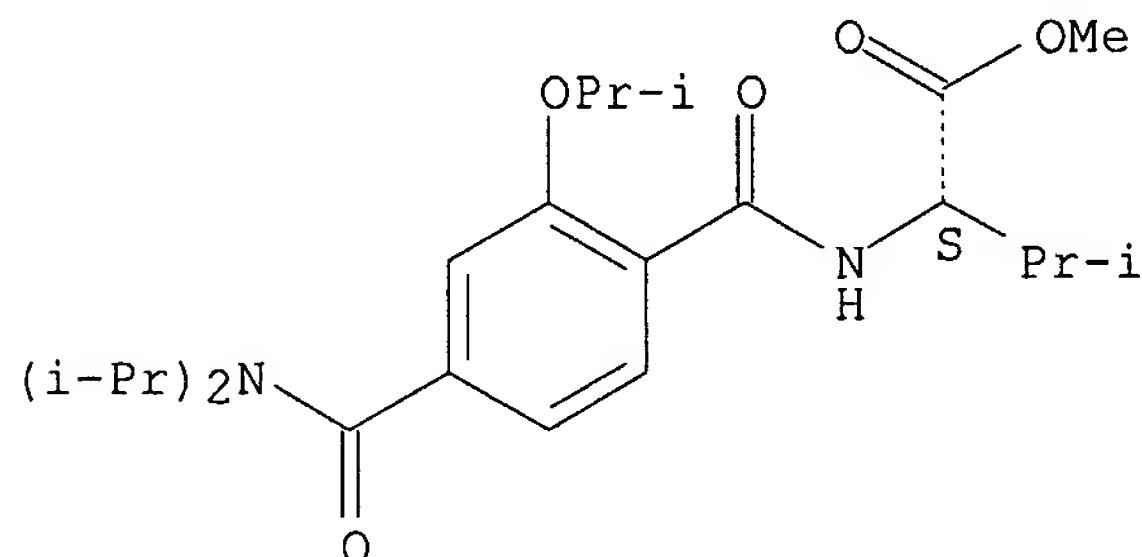
Absolute stereochemistry.



RN 681465-70-3 CAPLUS

CN L-Valine, N-[4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (CA INDEX NAME)

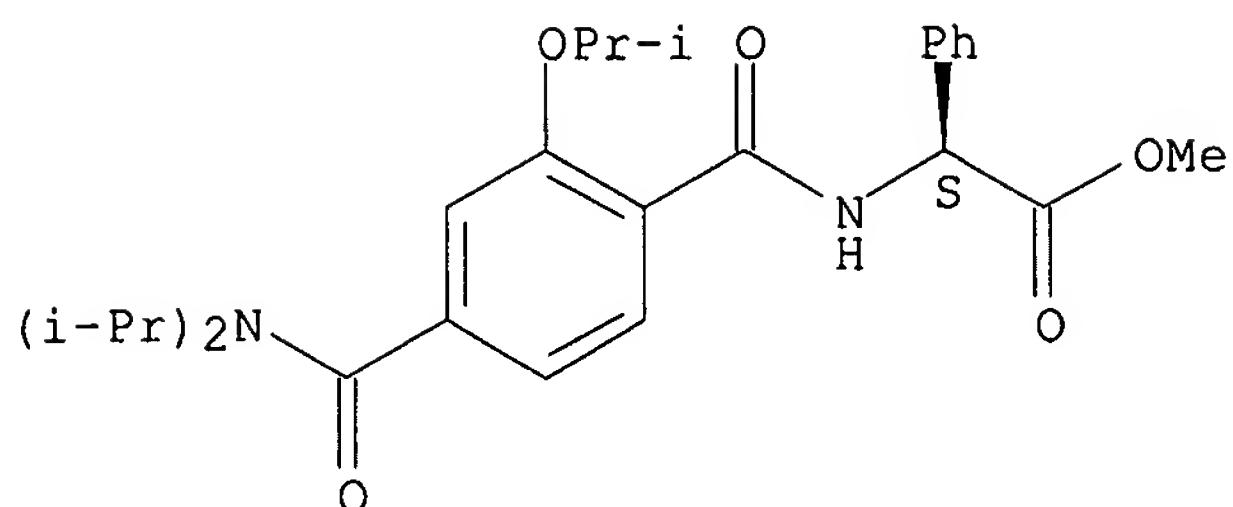
Absolute stereochemistry.



RN 681465-72-5 CAPLUS

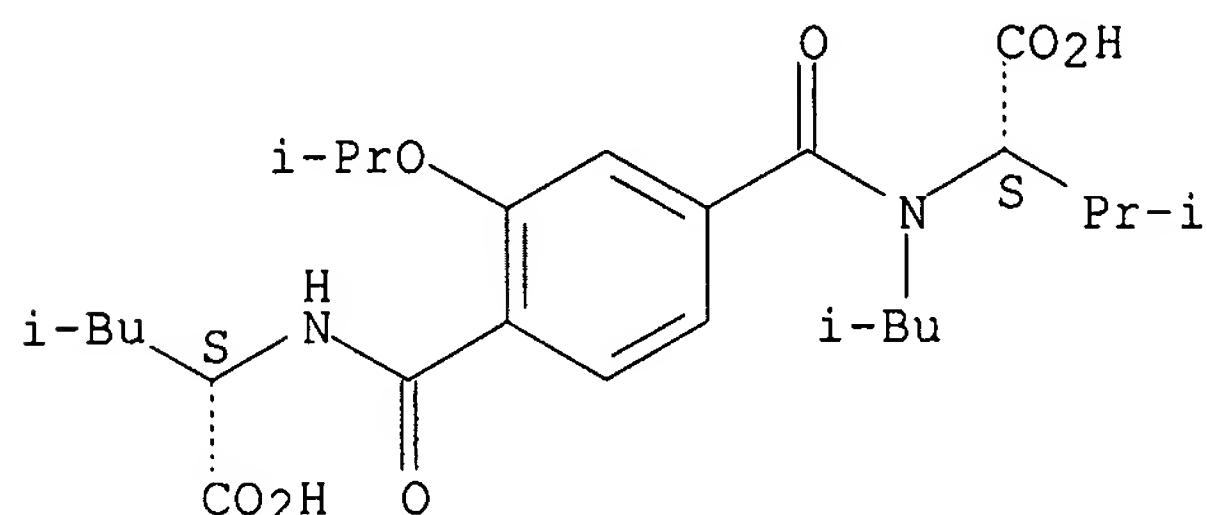
CN Benzeneacetic acid, alpha-[(4-[(bis(1-methylethyl)amino)carbonyl]-2-(1-methylethoxy)benzoyl]amino)-, methyl ester, (alphaS)- (CA INDEX NAME)

Absolute stereochemistry.



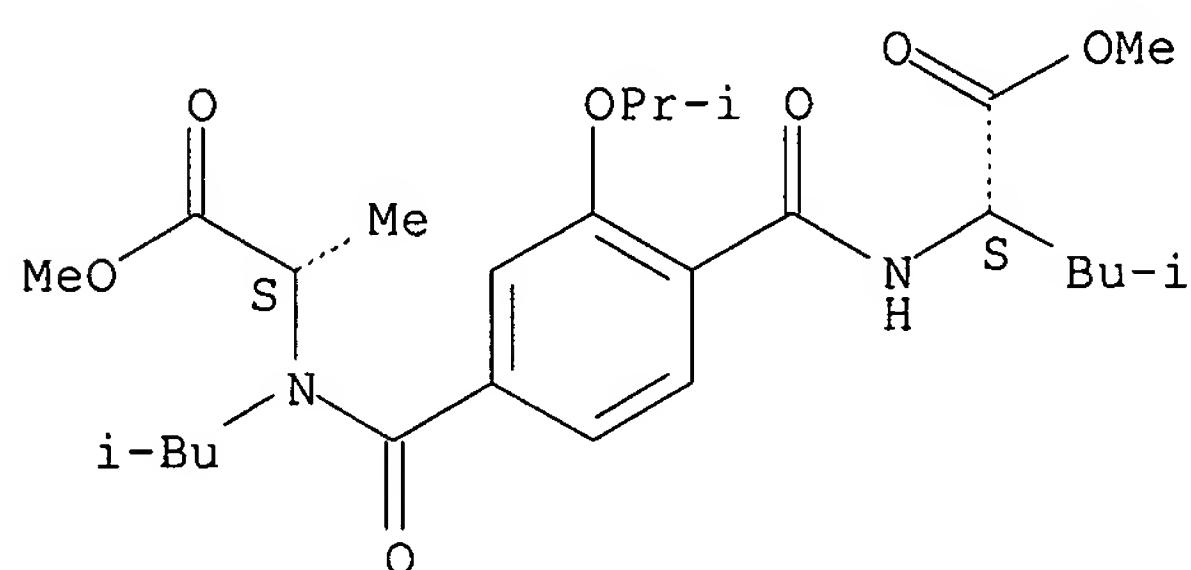
RN 681465-74-7 CAPLUS  
 CN L-Leucine, N-[4-[[[(1S)-1-carboxy-2-methylpropyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 681466-00-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (terephthalamide derivs. as novel Bcl-xL/Bak antagonists)  
 RN 681466-00-2 CAPLUS  
 CN L-Leucine, N-[4-[[[(1S)-2-methoxy-1-methyl-2-oxoethyl](2-methylpropyl)amino]carbonyl]-2-(1-methylethoxy)benzoyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

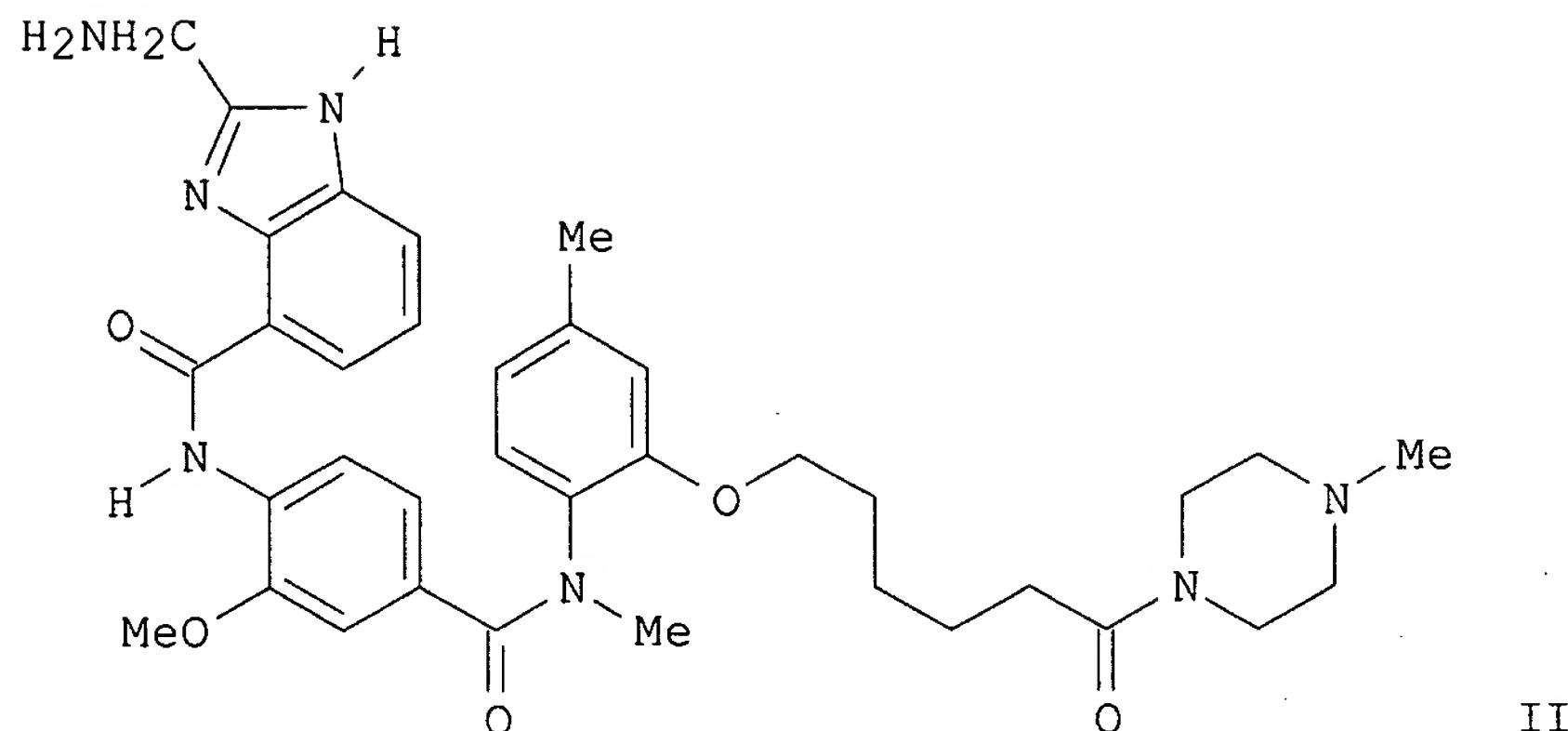
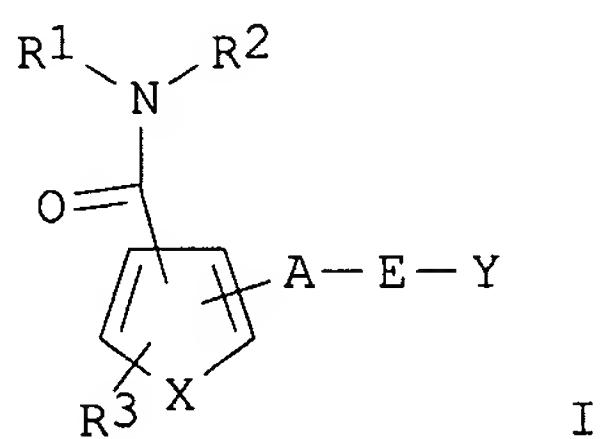


RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD  
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2008 ACS on STN  
 AN 1998:394328 CAPLUS  
 DN 129:67773  
 TI Preparation of benzamide derivatives having a vasopressin antagonistic activity  
 IN Setoi, Hiroyuki; Ohkawa, Takehiko; Zenkoh, Tatsuya; Sawada, Hitoshi;  
 Sawada, Yuki; Oku, Teruo  
 PA Fujisawa Pharmaceutical Co., Ltd., Japan  
 SO PCT Int. Appl., 332 pp.

CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

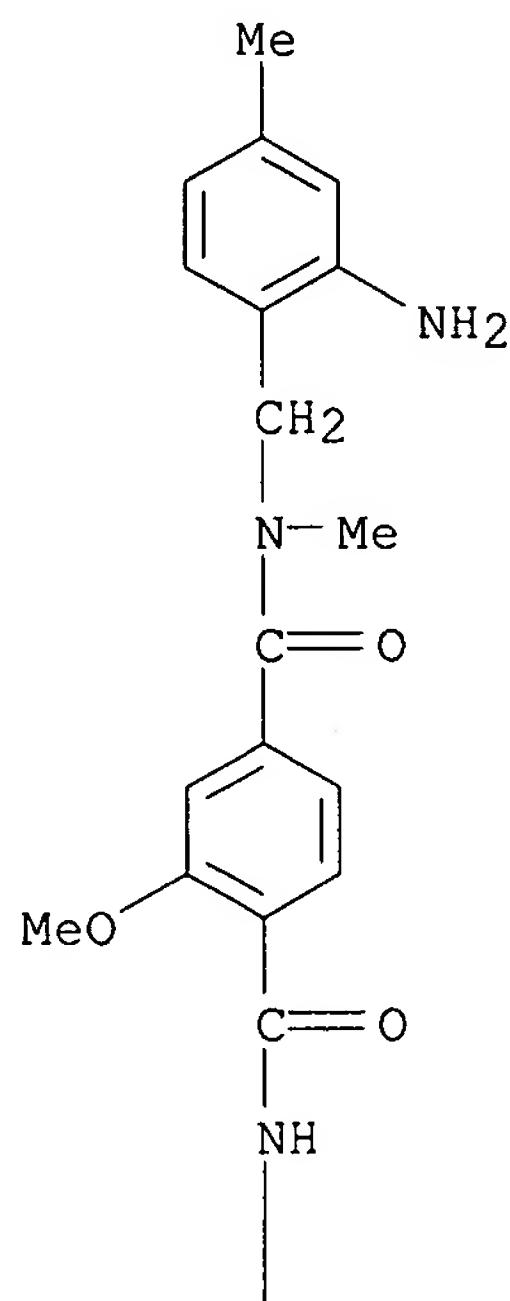
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9824771	A1	19980611	WO 1997-JP4192	19971118
	W: AU, CA, CN, HU, IL, JP, KR, MX, US, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE	
	AU 9749672	A	19980629	AU 1997-49672	19971118
	EP 946519	A1	19991006	EP 1997-912493	19971118
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
	JP 2001505193	T	20010417	JP 1998-521225	19971118
	US 6207693	B1	20010327	US 1999-308662	19990602
	US 6316482	B1	20011113	US 2000-614132	20000711
PRAI	AU 1996-3953	A	19961202		
	WO 1997-JP4192	W	19971118		
	US 1999-308662	A3	19990602		
OS	MARPAT 129:67773				
GI					



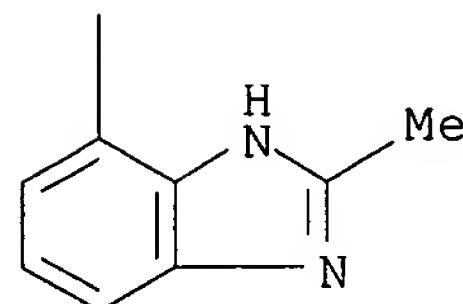
AB The title compds. [I; R1 = (un)substituted aryl, cyclo(lower)alkyl, heterocyclyl; R2 = H, lower alkyl, etc.; R3 = H, halo, OH, etc.; A = a single bond, O, NH; E = lower alkylene, lower alkenylene, etc.; X = CH:CH, CH:N, S; Y = (un)substituted aryl, condensed heterocyclyl, etc.] and their pharmaceutically acceptable salts, useful in treatment and/or prevention of hypertension, heart failure, renal insufficiency, edema, ascites, vasopressin parasecretion syndrome, hepatocirrhosis, hyponatremia, hypokalemia, diabetic, circulation disorder, cerebrovascular disease, Meniere's disease or motion sickness, were prepared. Thus, the title compound II showed IC50 of 1.5 nM against vasopressin 1 receptor binding.

IT 208770-26-7P  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of benzamide derivs. having a vasopressin antagonistic activity)  
RN 208770-26-7 CAPLUS  
CN 1,4-Benzenedicarboxamide, N4-[(2-amino-4-methylphenyl)methyl]-2-methoxy-N4-methyl-N1-(2-methyl-1H-benzimidazol-4-yl)-, dihydrochloride (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●2 HCl

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT